

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:spstasxml624

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	JAN 02	STN pricing information for 2008 now available
NEWS	3	JAN 16	CAS patent coverage enhanced to include exemplified prophetic substances
NEWS	4	JAN 28	USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS	5	JAN 28	MARPAT searching enhanced
NEWS	6	JAN 28	USGENE now provides USPTO sequence data within 3 days of publication
NEWS	7	JAN 28	TOXCENTER enhanced with reloaded MEDLINE segment
NEWS	8	JAN 28	MEDLINE and LMEEDLINE reloaded with enhancements
NEWS	9	FEB 08	STN Express, Version 8.3, now available
NEWS	10	FEB 20	PCI now available as a replacement to DPICI
NEWS	11	FEB 25	IFIREF reloaded with enhancements
NEWS	12	FEB 25	IMSPRODUCT reloaded with enhancements
NEWS	13	FEB 29	WPINDEX/WPIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification
NEWS	14	MAR 31	IFICDB, IFIPAT, and IFIUDB enhanced with new custom IPC display formats
NEWS	15	MAR 31	CAS REGISTRY enhanced with additional experimental spectra
NEWS	16	MAR 31	CA/CAPLUS and CASREACT patent number format for U.S. applications updated
NEWS	17	MAR 31	LPICI now available as a replacement to LDPCI
NEWS	18	MAR 31	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS	19	APR 04	STN AnaVist, Version 1, to be discontinued
NEWS	20	APR 15	WPIDS, WPINDEX, and WPIX enhanced with new predefined hit display formats
NEWS	21	APR 28	EMBASE Controlled Term thesaurus enhanced
NEWS	22	APR 28	IMSRSEARCH reloaded with enhancements
NEWS EXPRESS	FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3, AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008		
NEWS HOURS	STN Operating Hours Plus Help Desk Availability		
NEWS LOGIN	Welcome Banner and News Items		
NEWS IPC8	For general information regarding STN implementation of IPC 8		

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific

research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 16:57:10 ON 15 MAY 2008

=> fil reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 16:57:50 ON 15 MAY 2008  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 14 MAY 2008 HIGHEST RN 1020941-66-5  
DICTIONARY FILE UPDATES: 14 MAY 2008 HIGHEST RN 1020941-66-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

=>  
Uploading C:\Program Files\Stnexp\Queries\10584076.str



1

```
chain nodes :
17 20
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
ring bonds :
1-2 1-6 2-3 2-7 3-4 3-9 4-5 5-6 7-8 8-9 10-11 10-15 11-12 12-13 13-14
14-15
exact/norm bonds :
2-7 3-9 7-8 8-9
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15
```

G1:C,S,N

G2:Cy,Ak

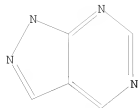
```
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 17:CLASS 18:Atom 20:CLASS
```

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

```
=> s ll sam
SAMPLE SEARCH INITIATED 16:58:05 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      2699 TO ITERATE

74.1% PROCESSED      2000 ITERATIONS      50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01
```

```
FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH  **COMPLETE**
PROJECTED ITERATIONS:   50864 TO   57096
PROJECTED ANSWERS:      37186 TO   42542
```

L2 50 SEA SSS SAM L1

```
=> log stng
'STNG' IS NOT VALID HERE
For an explanation, enter "HELP LOGOFF".
```

```
=> log h
COST IN U.S. DOLLARS      SINCE FILE      TOTAL
                           ENTRY      SESSION
FULL ESTIMATED COST      0.92      1.13
```

SESSION WILL BE HELD FOR 120 MINUTES  
STN INTERNATIONAL SESSION SUSPENDED AT 16:58:45 ON 15 MAY 2008

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssptasxm1624

```
PASSWORD:
* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'REGISTRY' AT 17:03:41 ON 15 MAY 2008
FILE 'REGISTRY' ENTERED AT 17:03:41 ON 15 MAY 2008
COPYRIGHT (C) 2008 American Chemical Society (ACS)
```

```
COST IN U.S. DOLLARS      SINCE FILE      TOTAL
                           ENTRY      SESSION
```

FULL ESTIMATED COST	0.92	1.13
=> fil reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.92	1.13

FILE 'REGISTRY' ENTERED AT 17:03:48 ON 15 MAY 2008  
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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 provided by InfoChem.

STRUCTURE FILE UPDATES: 14 MAY 2008 HIGHEST RN 1020941-66-5  
 DICTIONARY FILE UPDATES: 14 MAY 2008 HIGHEST RN 1020941-66-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when  
 conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and  
 predicted properties as well as tags indicating availability of  
 experimental property data in the original document. For information  
 on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10584076.str



```

chain nodes :
17 20
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
ring bonds :
1-2 1-6 2-3 2-7 3-4 3-9 4-5 5-6 7-8 8-9 10-11 10-15 11-12 12-13 13-14
14-15
exact/norm bonds :
2-7 3-9 7-8 8-9
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15

```

G1:C,S,N

G2:Cy,Ak

```

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 17:CLASS 18:Atom 20:CLASS

```

L3 STRUCTURE UPLOADED

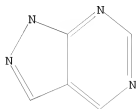
```

=> d
L3 HAS NO ANSWERS
L3 STR

```



G2



G1 C,S,N

G2 Cy,Ak

Structure attributes must be viewed using STN Express query preparation.

```

=> s l3 sam
SAMPLE SEARCH INITIATED 17:04:15 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2593 TO ITERATE

```

77.1% PROCESSED 2000 ITERATIONS 50 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 48806 TO 54914  
PROJECTED ANSWERS: 23621 TO 27927

L4 50 SEA SSS SAM L3

=> log h

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.46	1.59

SESSION WILL BE HELD FOR 120 MINUTES  
STN INTERNATIONAL SESSION SUSPENDED AT 17:04:32 ON 15 MAY 2008

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:spstasxml624

PASSWORD:

\* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \*  
SESSION RESUMED IN FILE 'REGISTRY' AT 17:06:06 ON 15 MAY 2008  
FILE 'REGISTRY' ENTERED AT 17:06:06 ON 15 MAY 2008  
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.46	1.59

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.46	1.59

FILE 'REGISTRY' ENTERED AT 17:06:15 ON 15 MAY 2008  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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STRUCTURE FILE UPDATES: 14 MAY 2008 HIGHEST RN 1020941-66-5  
DICTIONARY FILE UPDATES: 14 MAY 2008 HIGHEST RN 1020941-66-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

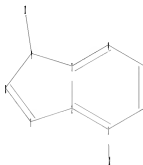
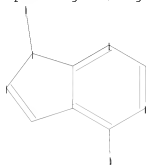
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

=>

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```
chain nodes :
12 13
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
1-12 9-13
ring bonds :
1-2 1-6 2-3 2-7 3-4 3-9 4-5 5-6 7-8 8-9
exact/norm bonds :
1-12 2-7 3-9 7-8 8-9 9-13
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
```

G1:C,S,N

G2:Cy,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 12:Atom  
13:Atom

L5 STRUCTURE UPLOADED

=> d

L5 HAS NO ANSWERS

L5 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.



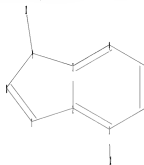
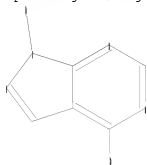
=> s 15 sam  
SAMPLE SEARCH INITIATED 17:06:54 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 19 TO ITERATE

100.0% PROCESSED 19 ITERATIONS 5 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 119 TO 641  
PROJECTED ANSWERS: 5 TO 234

L6 5 SEA SSS SAM L5

=>  
Uploading C:\Program Files\Stnexp\Queries\10584076a.str



chain nodes :  
12 13  
ring nodes :  
1 2 3 4 5 6 7 8 9  
chain bonds :  
1-12 9-13  
ring bonds :  
1-2 1-6 2-3 2-7 3-4 3-9 4-5 5-6 7-8 8-9  
exact/norm bonds :  
1-12 2-7 3-9 7-8 8-9 9-13  
normalized bonds :  
1-2 1-6 2-3 3-4 4-5 5-6

G1:C,S,N

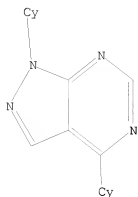
G2:Cy,Ak

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 12:Atom  
13:Atom

L7 STRUCTURE UPLOADED

=> d

L7 HAS NO ANSWERS  
L7 STR



G1 C,S,N

G2 Cy,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l7 sam

SAMPLE SEARCH INITIATED 17:07:48 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 2699 TO ITERATE

74.1% PROCESSED 2000 ITERATIONS

50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

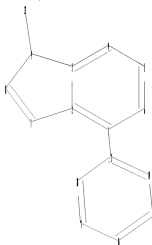
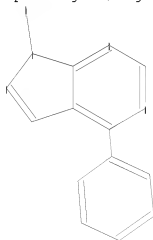
PROJECTED ITERATIONS: 50864 TO 57096

PROJECTED ANSWERS: 1675 TO 2967

L8 50 SEA SSS SAM L7

=>

Uploading C:\Program Files\Stnexp\Queries\10584076b.str



```

chain nodes :
12
ring nodes :
1 2 3 4 5 6 7 8 9 13 14 15 16 17 18
chain bonds :
1-13 9-12
ring bonds :
1-2 1-6 2-3 2-7 3-4 3-9 4-5 5-6 7-8 8-9 13-14 13-18 14-15 15-16 16-17
17-18
exact/norm bonds :
2-7 3-9 7-8 8-9 9-12
exact bonds :
1-13
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18

```

G1:C,S,N

G2:Cy,Ak

Match level :

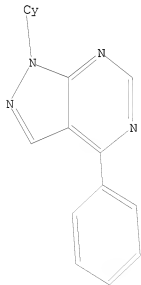
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 12:Atom  
13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom

L9 STRUCTURE UPLOADED

=> d

L9 HAS NO ANSWERS

L9 STR



G1 C,S,N

G2 Cy,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l9 sam

SAMPLE SEARCH INITIATED 17:11:25 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 48 TO ITERATE

100.0% PROCESSED 48 ITERATIONS 5 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 545 TO 1375  
PROJECTED ANSWERS: 5 TO 234

L10 5 SEA SSS SAM L9

=> s l9 ful

FULL SEARCH INITIATED 17:11:46 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 847 TO ITERATE

100.0% PROCESSED 847 ITERATIONS 115 ANSWERS  
SEARCH TIME: 00.00.01

L11 115 SEA SSS FUL L9

=> s l7 ful

FULL SEARCH INITIATED 17:12:52 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 54024 TO ITERATE

100.0% PROCESSED 54024 ITERATIONS 2254 ANSWERS  
SEARCH TIME: 00.00.02

L12 2254 SEA SSS FUL L7

=> fil capl

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
360.86	362.45

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 17:13:06 ON 15 MAY 2008

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FILE COVERS 1907 - 15 May 2008 VOL 148 ISS 20

FILE LAST UPDATED: 14 May 2008 (20080514/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.  
They are available for your review at:

<http://www.cas.org/legal/infopolicy.html>

=> s l12

L13            85 L12

=> s l13 not (2008/so or 2007/so ro 2006/so or 2005/so)

280963 2008/SO

922196 2007/SO

1501 SO/SO

157 RO/SO

942017 2006/SO

0 2007/SO RO 2006/SO

((2007(W) SO (W) RO (W) 2006) /SO)

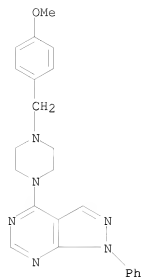
883097 2005/SO

L14            83 L13 NOT (2008/SO OR 2007/SO RO 2006/SO OR 2005/SO)

=> d l14 ibib hitstr abs 1-83

L14 ANSWER 1 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2008:352620 CAPLUS  
 DOCUMENT NUMBER: 148:369997  
 TITLE: Methods for identifying compounds that modulate BMP or  
 TGF- $\beta$  cell signaling and methods employing such  
 compounds  
 INVENTOR(S): Yu, Paul B.; Hong, Charles C.; Bloch, Kenneth D.;  
 Peterson, Randall T.  
 PATENT ASSIGNEE(S): The General Hospital Corporation, USA  
 SOURCE: PCT Int. Appl., 78pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008033408	AZ	20080320	WO 2007-US19831	20070912
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
PRIORITY APPLN. INFO.:			US 2006-844038P	P 20060912
IT 612038-02-5				
RL:	PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)			
	(methods for identifying compds. that modulate BMP or TGF- $\beta$ cell signaling, and therapeutic methods)			
RN 612038-02-5	CAPLUS			
CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[4-[(4-methoxyphenyl)methyl]-1-piperazinyl]-1-phenyl-	(CA INDEX NAME)			



AB The invention provides methods for identifying compds. that modulate bone morphogenetic protein (BMP) or transforming growth factor- $\beta$  (TGF- $\beta$ ) cell signaling, as well as therapeutic methods that employ such compds.

ACCESSION NUMBER: 2007:1395576 CAPLUS

DOCUMENT NUMBER: 148:33757

TITLE: Preparation of substituted pyrazolopyrimidines as inhibitors of glycogen synthase kinase 3 and cyclin dependent kinase 5

INVENTOR(S): Bacon, Edward R.; Bailey, Thomas; Becknell, Nadine C.; Gingrich, Diane E.; Hostetler, Greg; Hudkins, Robert L.; Learn, Keith S.; Wagner, Jason C.

PATENT ASSIGNEE(S): Cephalon, Inc., USA

SOURCE: U.S. Pat. Appl. Publ., 120pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20070281949	A1	20071206	US 2007-803320	20070514
PRIORITY APPLN. INFO.:			US 2006-800375P	P 20060515
OTHER SOURCE(S): MARPAT 148:33757				
IT 959430-43-4P, 5-Bromo-3-(1-cyclopentyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-1,3-dihydroindol-2-one 959430-44-5P, 3-(1-Cyclopentyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-2-oxo-2,3-dihydro-1H-indole-5-carbonitrile 959430-45-6P 959430-46-7P, 3-(1-Cyclopentyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-5-nitro-1,3-dihydroindol-2-one 959430-47-8P, 5-Chloro-3-(1-cyclopentyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-1,3-dihydroindol-2-one 959430-48-9P, 6-Chloro-3-(1-cyclopentyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-1,3-dihydroindol-2-one 959430-49-0P, 3-(1-Cyclopentyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-5,7-dinitro-1,3-dihydroindol-2-one 959430-50-3P, 3-(1-Cyclopentyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-5,7-difluoro-1,3-dihydroindol-2-one 959430-51-4P, 3-(1-Cyclopentyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-1,3-dihydroindol-2-one 959430-52-5P, 3-(1-Cyclopentyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-2-oxo-2,3-dihydro-1H-indole-6-carbonitrile 959430-53-6P, 3-(1-Cyclopentyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-2-oxo-2,3-dihydro-1H-indole-7-carbonitrile 959430-54-7P, 3-(1-Cyclopentyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-5-fluoro-1,3-dihydroindol-2-one 959430-55-8P, 3-(1-Cyclopentyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-6-fluoro-1,3-dihydroindol-2-one 959430-56-9P, 3-(1-Cyclopentyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-4,5-difluoro-1,3-dihydroindol-2-one 959430-57-0P, 3-(1-Cyclohexyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-2-oxo-2,3-dihydro-1H-indole-5-carbonitrile 959430-58-1P, 3-(1-Cyclohexyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-2-oxo-2,3-dihydro-1H-indole-6-carbonitrile 959430-59-2P, 3-(1-Cyclohexyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-2-oxo-2,3-dihydro-1H-indole-7-carbonitrile 959430-60-5P, 3-(1-Cyclohexyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-5-trifluoromethyl-1,3-dihydroindol-2-one 959430-61-6P, 3-(1-Cyclohexyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-5-fluoro-1,3-dihydroindol-2-one 959430-62-7P, 3-(1-Cyclohexyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-6-fluoro-1,3-dihydroindol-2-one 959430-63-8P, 5-Chloro-3-(1-Cyclohexyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-1,3-dihydroindol-2-one 959430-64-9P, 5-Bromo-3-(1-Cyclohexyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-1,3-dihydroindol-2-one				

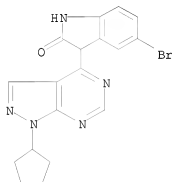
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)



(drug candidate; preparation of substituted pyrazolopyrimidines as inhibitors of glycogen synthase kinase 3 and cyclin dependent kinase 5)

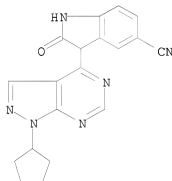
RN 959430-43-4 CAPLUS

CN 2H-Indol-2-one, 5-bromo-3-(1-cyclopentyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-1,3-dihydro- (CA INDEX NAME)



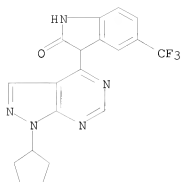
RN 959430-44-5 CAPLUS

CN 1H-Indole-5-carbonitrile, 3-(1-cyclopentyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-2,3-dihydro-2-oxo- (CA INDEX NAME)



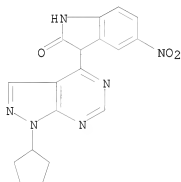
RN 959430-45-6 CAPLUS

CN 2H-Indol-2-one, 3-(1-cyclopentyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-1,3-dihydro-5-(trifluoromethyl)- (CA INDEX NAME)



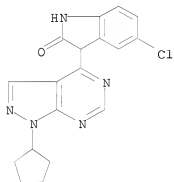
RN 959430-46-7 CAPLUS

CN 2H-Indol-2-one, 3-(1-cyclopentyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-1,3-dihydro-5-nitro- (CA INDEX NAME)



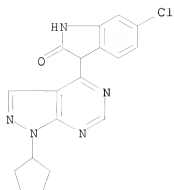
RN 959430-47-8 CAPLUS

CN 2H-Indol-2-one, 5-chloro-3-(1-cyclopentyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-1,3-dihydro- (CA INDEX NAME)



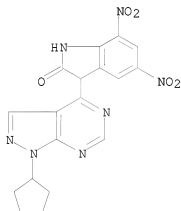
RN 959430-48-9 CAPLUS

CN 2H-Indol-2-one, 6-chloro-3-(1-cyclopentyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-1,3-dihydro- (CA INDEX NAME)



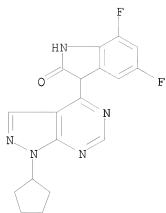
RN 959430-49-0 CAPLUS

CN 2H-Indol-2-one, 3-(1-cyclopentyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-1,3-dihydro-5,7-dinitro- (CA INDEX NAME)



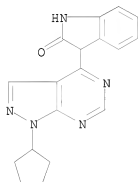
RN 959430-50-3 CAPLUS

CN 2H-Indol-2-one, 3-(1-cyclopentyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-5,7-difluoro-1,3-dihydro- (CA INDEX NAME)



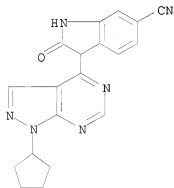
RN 959430-51-4 CAPLUS

CN 2H-Indol-2-one, 3-(1-cyclopentyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-1,3-dihydro- (CA INDEX NAME)



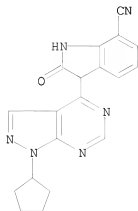
RN 959430-52-5 CAPLUS

CN 1H-Indole-6-carbonitrile, 3-(1-cyclopentyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-2,3-dihydro-2-oxo- (CA INDEX NAME)



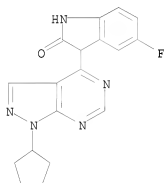
RN 959430-53-6 CAPLUS

CN 1H-Indole-7-carbonitrile, 3-(1-cyclopentyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-2,3-dihydro-2-oxo- (CA INDEX NAME)



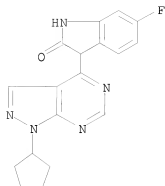
RN 959430-54-7 CAPLUS

CN 2H-Indol-2-one, 3-(1-cyclopentyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-5-fluoro-1,3-dihydro- (CA INDEX NAME)



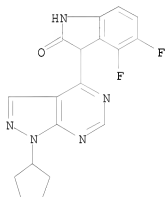
RN 959430-55-8 CAPLUS

CN 2H-Indol-2-one, 3-(1-cyclopentyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-6-fluoro-1,3-dihydro- (CA INDEX NAME)



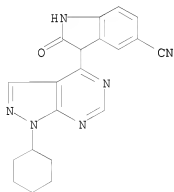
RN 959430-56-9 CAPLUS

CN 2H-Indol-2-one, 3-(1-cyclopentyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-4,5-difluoro-1,3-dihydro- (CA INDEX NAME)



RN 959430-57-0 CAPLUS

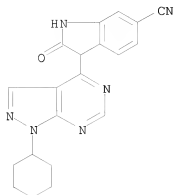
CN 1H-Indole-5-carbonitrile, 3-(1-cyclohexyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-2,3-dihydro-2-oxo- (CA INDEX NAME)



RN 959430-58-1 CAPLUS

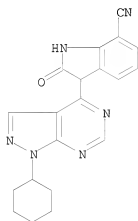
CN 1H-Indole-6-carbonitrile, 3-(1-cyclohexyl-1H-pyrazolo[3,4-d]pyrimidin-4-

yl)-2,3-dihydro-2-oxo- (CA INDEX NAME)



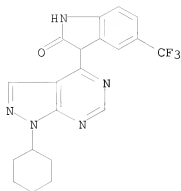
RN 959430-59-2 CAPLUS

CN 1H-Indole-7-carbonitrile, 3-(1-cyclohexyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-2,3-dihydro-2-oxo- (CA INDEX NAME)

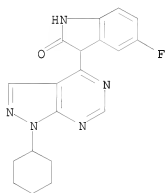


RN 959430-60-5 CAPLUS

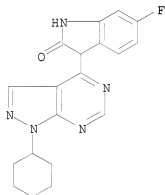
CN 2H-Indol-2-one, 3-(1-cyclohexyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-1,3-dihydro-5-(trifluoromethyl)- (CA INDEX NAME)



RN 959430-61-6 CAPLUS  
 CN 2H-Indol-2-one, 3-(1-cyclohexyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-5-fluoro-  
 1,3-dihydro- (CA INDEX NAME)



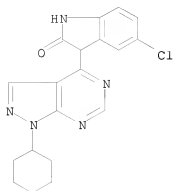
RN 959430-62-7 CAPLUS  
 CN 2H-Indol-2-one, 3-(1-cyclohexyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-6-fluoro-  
 1,3-dihydro- (CA INDEX NAME)



RN 959430-63-8 CAPLUS  
 CN 2H-Indol-2-one, 5-chloro-3-(1-cyclohexyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-  
 1,3-dihydro- (CA INDEX NAME)

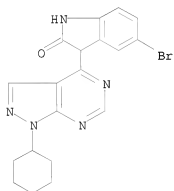


1,3-dihydro- (CA INDEX NAME)

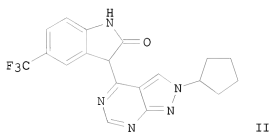
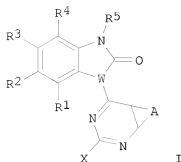


RN 959430-64-9 CAPLUS

CN 2H-Indol-2-one, 5-bromo-3-(1-cyclohexyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-  
1,3-dihydro- (CA INDEX NAME)



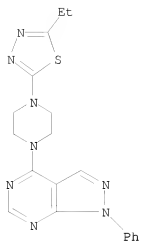
GI



AB The invention is related to substituted heterobicyclic pyrimidines I [W = CH, N; A = (un)substituted 3,4-1H-pyrazolylene, 3,4-2H-pyrazolylene, 4,5-1H-4,5-triazolylene, 1,2-cyclohex-1-enylene, 2,3-pyridinylen, etc.; R1-R4 = independently H, halo, NO2, CN, CF3, NH2 and derivs., SO2NH2 and derivs., NHC(=O)2H and derivs., etc.; R5 = H, alkyl, or a prodrug of an amino group; X = H, NH2 and derivs., alk(en/yn)yl, SH and derivs., OCONH2 and derivs., etc.], especially pyrazolopyrimidines, their stereoisomers, tautomers, prodrugs, and pharmaceutically acceptable salts, to pharmaceutical compns. containing them and to their use as inhibitors of glycogen synthase kinase 3 (GSK3) and cyclin dependent kinase 5 (CDK5) in the treatment of chronic neurodegenerative diseases, neurotraumatic diseases, depression and/or diabetes. Thus, hydration of 3-amino-1-cyclopentyl-1H-pyrazole-4-carbonitrile (preparation given), cyclization of amino pyrazolecarboxamide with formamidine acetate, aromatization of 2-cyclopentyl-2,5-dihydropyrazolo[3,4-d]pyrimidin-4-one by treatment with POC13 and reaction of the chloride with 5-cyanooxindole gave pyrazolopyrimidine II. Pyrazolopyrimidine II inhibited CDK5 and GSK3 $\beta$  kinases with IC50 < 300 nM.

L14 ANSWER 3 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2007:1023400 CAPLUS  
 DOCUMENT NUMBER: 147:357124  
 TITLE: Use of inhibitors of scavenger receptor class proteins  
 for the treatment of infectious diseases  
 INVENTOR(S): Hannus, Michael; Martin, Cecillie; Mota, Maria M.;  
 Prudencio, Miguel; Rodrigues, Christina Dias  
 PATENT ASSIGNEE(S): Cenix Bioscience G.m.b.H., Germany; Instituto de  
 Medicina Molecular, Faculdade de Medicina da  
 Universidade de Lisboa  
 SOURCE: PCT Int. Appl., 127pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007101710	A1	20070913	WO 2007-EP2110	20070309
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
EP 1832283	A1	20070912	EP 2006-4854	20060309
R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU			
PRIORITY APPLN. INFO.:			EP 2006-4854	A 20060309
			US 2006-780567P	P 20060309
OTHER SOURCE(S):	MARPAT 147:357124			
IT 313364-25-9				
RL:	PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)			
	(use of inhibitors of scavenger receptor class proteins for treatment of infectious diseases)			
RN 313364-25-9	CAPLUS			
CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[4-(5-ethyl-1,3,4-thiadiazol-2-yl)-1-piperazinyl]-1-phenyl-	(CA INDEX NAME)			

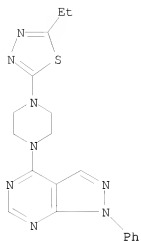


AB The invention relates to the use of inhibitors of scavenger receptor class proteins, in particular ScarB1 for the production of a medicament for treatment of and/or prophylaxis against infections, involving liver cells and/or hematopoietic cells, in particular malaria. Administration of ezetimibe to mice injected with *Plasmodium berghei* significantly reduced liver infection rate. Small interfering RNAs targeting ScarB1 reduced EEf (Exo-Erythrocytic Form) development in human hepatoma cells infected with *Plasmodium berghei* sporozoites.

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 4 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2007:1018595 CAPLUS  
 DOCUMENT NUMBER: 147:357121  
 TITLE: Use of inhibitors of scavenger receptor class proteins  
 for the treatment of infectious diseases  
 INVENTOR(S): Hannus, Michael; Martin, Cecilie; Mota, Maria M.;  
 Prudencio, Miguel; Rodrigues, Christina Dias  
 PATENT ASSIGNEE(S): Cenix Bioscience GmbH, Germany; Instituto De Medicina  
 Molecular  
 SOURCE: Eur. Pat. Appl., 66pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1832283	A1	20070912	EP 2006-4854	20060309
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU				
WO 2007101710	A1	20070913	WO 2007-EP2110	20070309
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
PRIORITY APPLN. INFO.:			EP 2006-4854	A 20060309
			US 2006-780567P	P 20060309
OTHER SOURCE(S):		MARPAT 147:357121		
IT 313364-25-9				
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (use of inhibitors of scavenger receptor class proteins for treatment of infectious diseases)				
RN 313364-25-9 CAPLUS				
CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[4-(5-ethyl-1,3,4-thiadiazol-2-yl)-1- piperazinyl]-1-phenyl- (CA INDEX NAME)				



AB The invention relates to the use of inhibitors of scavenger receptor class proteins, in particular ScarB1 for the production of a medicament for treatment of and/or prophylaxis against infections, involving liver cells and/or hematopoietic cells, in particular malaria. Administration of ezetimibe to mice injected with *Plasmodium berghei* significantly reduced liver infection rate. Small interfering RNAs targeting ScarB1 reduced EEF (Exo-Erythrocytic Form) development in human hepatoma cells infected with *Plasmodium berghei* sporozoites.

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 5 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:970312 CAPLUS

DOCUMENT NUMBER: 147:269256

TITLE: Drug compositions containing pyrazolopyrimidine derivatives

INVENTOR(S): Takamuro, Iwao; Kanan, Saburo; Tsuboi, Yasunori; Mochida, Hideki; Noshiro, Hiroshi

PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 51pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2007217407	A	20070830	JP 2007-8617	20070118
PRIORITY APPLN. INFO.:			JP 2006-10570	A 20060119

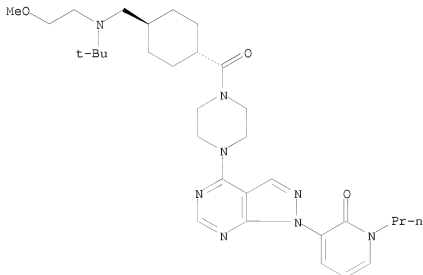
OTHER SOURCE(S): MARPAT 147:269256

IT 874382-15-7, 1-(2-Oxo-1-propyl-1,2-dihydropyridin-3-yl)-4-[4-  
[[trans-4-[[N-tert-butyl-(2-methoxyethyl)amino]methyl]cyclohexyl]carbonyl]  
piperazin-1-yl]-1H-pyrazolo[3,4-d]pyrimidine 874382-16-8,  
1-(2-Oxo-1-propyl-1,2-dihydropyridin-3-yl)-4-[4-[(trans-4-piperidin-1-  
ylcyclohexyl)carbonyl]piperazin-1-yl]-1H-pyrazolo[3,4-d]pyrimidine  
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL  
(Biological study); USES (Uses)  
(drug comps. containing pyrazolopyrimidine derivs. as SK channel blockers)

RN 874382-15-7 CAPLUS

CN 2(1H)-Pyridinone, 3-[4-[4-[[trans-4-[[[1,1-dimethylethyl](2-  
methoxyethyl)amino]methyl]cyclohexyl]carbonyl]-1-piperazinyl]-1H-  
pyrazolo[3,4-d]pyrimidin-1-yl]-1-propyl- (CA INDEX NAME)

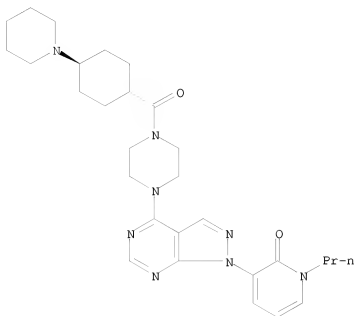
Relative stereochemistry.



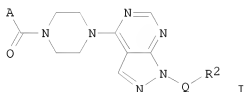
RN 874382-16-8 CAPLUS

CN 2(1H)-Pyridinone, 3-[4-[4-[[trans-4-(1-piperidinyl)cyclohexyl]carbonyl]-1-  
piperazinyl]-1H-pyrazolo[3,4-d]pyrimidin-1-yl]-1-propyl- (CA INDEX NAME)

Relative stereochemistry.



GI



AB Disclosed are drug compns. characterized by containing pyrazolopyrimidine derivs. represented by a general formula I (A = amino-containing alkyl-substituted cyclohexyl or piperidyl; R<sub>2</sub> = substituted benzyl, substituted pyridyl, substituted thiazolyl, etc.), or its pharmaceutically acceptable salt as an active component. The compound has SK channel-blocking effect, and is suitable for use for treatment of digestive tract disorder, central nervous system disease, tonic muscular dystrophy, bladder disorder, etc. For example, 1-(3-Ethoxybenzyl)-4-[4-[[4-[N-(2-methoxyethyl)-N-(tert-butyl)aminomethyl]piperidin-1-yl]carbonyl]piperazin-1-yl]-1H-pyrazolo[3,4-d]pyrimidine hydrochloride was prepared, and examined for its effect against SK channel in vitro.



ACCESSION NUMBER: 2007:849780 CAPLUS

DOCUMENT NUMBER: 148:115389

TITLE: Virtual screening of tubercular acetohydroxy acid synthase inhibitors through analysis of structural models

AUTHOR(S): Le, Dung Tien; Lee, Hyun-Sook; Chung, Young-Je; Yoon, Moon-Young; Choi, Jung-Do

CORPORATE SOURCE: School of Life Sciences, Chungbuk National University, Cheongju, 361-763, S. Korea

SOURCE: Bulletin of the Korean Chemical Society (2007), 28(6), 947-952

CODEN: BKCSDE; ISSN: 0253-2964

PUBLISHER: Korean Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

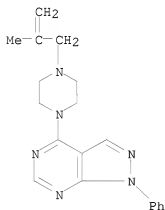
IT 331761-36-5

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(All 50 compds., Table 4, page 951; binding to tubercular acetohydroxy acid synthase)

RN 331761-36-5 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[4-(2-methyl-2-propen-1-yl)-1-piperazinyl]-1-phenyl- (CA INDEX NAME)



AB Mycobacterium tuberculosis is a pathogen responsible for 2-3 million deaths every year worldwide. The emergence of drug-resistant and multidrug-resistant tuberculosis has increased the need to identify new antituberculosis targets. Acetohydroxy acid synthase, (AHAS, EC 2.2.1.6), an enzyme involved in branched-chain amino acid synthesis, has recently been identified as a potential anti-tuberculosis target. To assist in the search for new inhibitors and "receptor-based" design of effective inhibitors of tubercular AHAS (TbAHAS), we constructed four different structural models of TbAHAS and used one of the models as a target for virtual screening of potential inhibitors. The quality of each model was assessed stereochem. by PROCHECK and found to be reliable. Up to 89% of the amino acid residues in the structural models were located in the most favored regions of the Ramachandran plot, which indicates that the conformation of each residue in the models is good. In the models, residues at the herbicide-binding site were highly conserved across 39 AHAS sequences. The binding mode of TbAHAS with a sulfonylurea herbicide

was characterized by 32 hydrophobic interactions, the majority of which were contributed by residue Trp516. The model based on the highest resolution X-ray structure of yeast AHAS was used as the target for virtual screening of a chemical database containing 8300 mols. with a heterocyclic ring.

We developed a short list of mols. that were predicted to bind with high scores to TbaHAS in a conformation similar to that of sulfonylurea derivs. Five sulfonylurea herbicides that were calculated to efficiently bind TbaHAS were exptl. verified and found to inhibit enzyme activity at micromolar concns. The data suggest that this time-saving and cost-effective computational approach can be used to discover new TbaHAS inhibitors. The list of chems. studied in this work is supplied to facilitate independent exptl. verification of the computational approach.

REFERENCE COUNT:        44        THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 7 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:158018 CAPLUS

DOCUMENT NUMBER: 147:406787

TITLE: Condensed pyrimidine systems. 4. Synthesis and transformations of 6-(trifluoromethyl)-1H-pyrazolo[3,4-d]pyrimidin-4(5H)-ones

AUTHOR(S): Bol'but, A. V.; Korol'ov, O. K.; Vovk, M. V.

CORPORATE SOURCE: Inst. Org. Khim., NAN Ukraini, Kiev, 02094, Ukraine

SOURCE: Zhurnal Organichnoi ta Farmatsevtichnoi Khimii (2006), 4(1), 66-69

CODEN: ZOFKAM

PUBLISHER: Natsional'nii Farmatsevtichnii Universitet

DOCUMENT TYPE: Journal

LANGUAGE: Ukrainian

OTHER SOURCE(S): CASREACT 147:406787

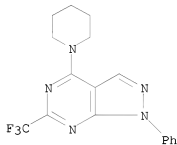
IT 871547-68-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of trifluoromethyl-substituted pyrazolo- and pyrazolo-tetrazolo pyrimidinones and their derivs. by heterocyclization of aminopyrazole carboxamide with trifluoroacetate)

RN 871547-68-1 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-phenyl-4-(1-piperidinyl)-6-  
(trifluoromethyl)- (CA INDEX NAME)



AB 1-R-6-Trifluoromethyl-1H-pyrazolo[3,4-d]pyrimidin-4(5H)-ones (2a-d; R = Me, PhCH<sub>2</sub>, Ph, 3-ClC<sub>6</sub>H<sub>4</sub>) were prepared by heterocyclization of 5-aminopyrazole-4-carboxamides with Me trifluoroacetate. The pyrimidinones 2 were converted into the corresponding 4-alkoxy, chloro, amino and hydrazino derivs. and 7-R-5-trifluoromethyl-7H-pyrazolo[4,3-e]tetrazolo[1,5-c]pyrimidines (7a-c; R = PhCH<sub>2</sub>, Ph, 3-ClC<sub>6</sub>H<sub>4</sub>).

L14 ANSWER 8 OF 83 CAPLUS COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 2006:79406 CAPLUS

DOCUMENT NUMBER: 144:171006

TITLE: Preparation of pyrazolopyrimidines and related compounds as SK channel blockers

INVENTOR(S): Takamuro, Iwao; Kawanami, Saburo; Tsuboi, Yasunori; Himiyama, Toshiyuki; Miura, Yuko; Mochida, Hideki; Nogi, Kouji

PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan

SOURCE: PCT Int. Appl., 126 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

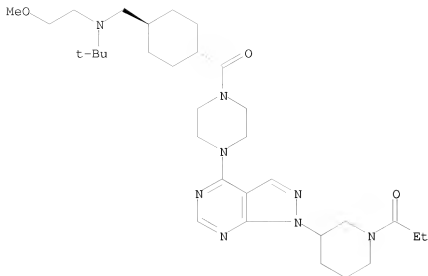
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006009245	A1	20060126	WO 2005-JP13459	20050722
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TG, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
JP 2006056882	A	20060302	JP 2005-210976	20050721
JP 2006056883	A	20060302	JP 2005-210977	20050721
EP 1772454	A1	20070411	EP 2005-766456	20050722
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU				
CN 101023083	A	20070822	CN 2005-80031675	20050722
US 20080081817	A1	20080403	US 2007-632725	20070326
PRIORITY APPLN. INFO.:			JP 2004-216500	A 20040723
			JP 2004-216501	A 20040723
			WO 2005-JP13459	W 20050722

OTHER SOURCE(S): MARPAT 144:171006

IT 874382-13-5 874382-15-7, 1-(2-Oxo-1-propyl-1,2-dihydropyridin-3-yl)-4-[4-[[trans-4-[[N-tert-butyl-(2-methoxyethyl)amino]methyl]cyclohexyl]carbonyl]piperazin-1-yl]-1H-pyrazolo[3,4-d]pyrimidine 874382-16-8, 1-(2-Oxo-1-propyl-1,2-dihydropyridin-3-yl)-4-[4-[[trans-4-(piperidin-1-yl)cyclohexyl]carbonyl]piperazin-1-yl]-1H-pyrazolo[3,4-d]pyrimidine  
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (preparation of pyrazolopyrimidines and related compds. as SK channel blockers)  
 RN 874382-13-5 CAPLUS  
 CN 1-Propanone, 1-[3-[4-[4-[[trans-4-[[1,1-dimethylethyl](2-methoxyethyl)amino]methyl]cyclohexyl]carbonyl]-1-piperazinyl]-1H-pyrazolo[3,4-d]pyrimidin-1-yl]-1-piperidinyl- (CA INDEX NAME)

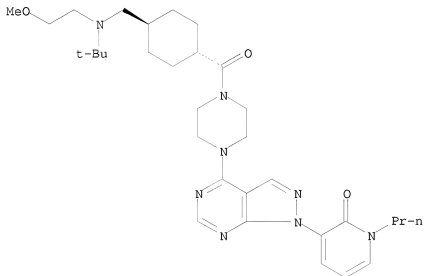
Relative stereochemistry.



RN 874382-15-7 CAPLUS

CN 2-(1H)-Pyridinone, 3-[4-[4-[[trans-4-[(1,1-dimethylethyl)(2-methoxyethyl)amino]methyl]cyclohexyl]carbonyl]-1-piperazinyl]-1H-pyrazolo[3,4-d]pyrimidin-1-yl]-1-propyl- (CA INDEX NAME)

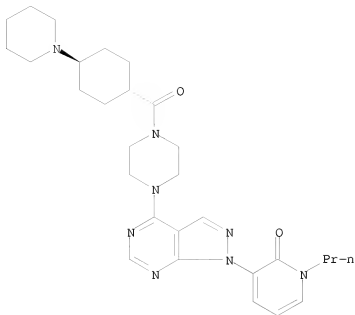
Relative stereochemistry.



RN 874382-16-8 CAPLUS

CN 2-(1H)-Pyridinone, 3-[4-[4-[[trans-4-(1-piperidinyl)cyclohexyl]carbonyl]-1-piperazinyl]-1H-pyrazolo[3,4-d]pyrimidin-1-yl]-1-propyl- (CA INDEX NAME)

Relative stereochemistry.



GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Title compds. I [R0 = H, halo, cyano, etc.; R1 = Q1, Q2; R11, R12 = H, alkyl, hydroxyalkyl, etc.; X = N, CH; m = 0, 1; A = -(NH)n-Alk-NH-, Q3, Q4; when one of X1 and X2 is CH or N, the other is N; Alk = alkylene; n = 0, 1; D1, D2, D3 = N, CH; R2 = halo, optionally substituted alkyl with halo, optionally substituted alkoxy with halo, etc.; R3 = H, alkyl; Q = alkylene] were prepared For example, EDCI mediated amidation of trans-4-(piperidin-1-yl)cyclohexanecarboxylic acid hydrochloride, e.g., prepared from trans-cyclohexane-1,4-dicarboxylic acid in 6 steps, with 6-chloro-1-(3-ethoxybenzyl)-4-(piperazin-1-yl)-1H-pyrazolo[3,4-d]pyrimidine·2HCl followed by treatment with HCl afforded compound II hydrochloride. Compds. I are claimed useful for the treatment of diseases related to SK channel (no data).

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 9 OF 83 CAPLUS COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 2005:1314205 CAPLUS

DOCUMENT NUMBER: 144:51610

TITLE: Preparation and structure activity of pyrazolo-pyrimidine derivatives as antitumor agents and kinase modulators

INVENTOR(S): Anand, Neel K.; Blazey, Charles M.; Bowles, Owen Joseph; Bussenius, Joerg; Canne Bannen, Lynne; Chan, Diva Sze-Ming; Chen, Baili; Co, Erick Wang; Costanzo, Simona; Defina, Steven Charles; Dubenko, Larisa; Franzini, Maurizio; Huang, Ping; Jammalamadaka, Vasu; Khoury, Richard George; Kim, Moon Hwan; Klein, Rhett Ronald; Le, Donna Tra; Mac, Morrison B.; Nuss, John M.; Parks, Jason Jevious; Rice, Kenneth D.; Tsang, Tsze H.; Tshako, Amy Lew; Wang, Yong; Xu, Wei

PATENT ASSIGNEE(S): Exelixis, Inc., USA  
SOURCE: PCT Int. Appl., 211 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005117909	A2	20051215	WO 2005-US13860	20050422
WO 2005117909	A3	20060427		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2005249380	A1	20051215	AU 2005-249380	20050422
CA 2563699	A1	20051215	CA 2005-2563699	20050422
EP 1750727	A2	20070214	EP 2005-804792	20050422
R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU			
JP 2007534687	T	20071129	JP 2007-509678	20050422
US 20080076774	A1	20080327	US 2007-568173	20070726
PRIORITY APPLN. INFO.:			US 2004-564908P	P 20040423
			WO 2005-US13860	W 20050422

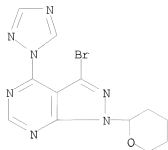
OTHER SOURCE(S): CASREACT 144:51610; MARPAT 144:51610

IT 871341-91-2

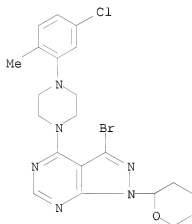
RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation and structure activity of pyrazolopyrimidine derivs. as antitumor agents and kinase modulators)

RN 871341-91-2 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 3-bromo-1-(tetrahydro-2H-pyran-2-yl)-4-(1H-1,2,4-triazol-1-yl)- (CA INDEX NAME)



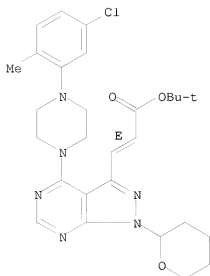
IT 871338-04-4P 871338-05-5P 871338-27-1P  
 871338-28-2P 871338-29-3P 871338-30-6P  
 871338-37-3P 871340-51-1P 871340-77-1P  
 871341-92-3P 871341-93-4P 871341-95-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and structure activity of pyrazolopyrimidine derivs. as  
 antitumor agents and kinase modulators)  
 RN 871338-04-4 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 3-bromo-4-[4-(5-chloro-2-methylphenyl)-1-  
 piperazinyl]-1-(tetrahydro-2H-pyran-2-yl)- (CA INDEX NAME)



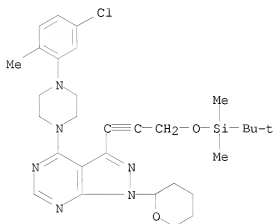
RN 871338-05-5 CAPLUS  
 CN 2-Propenoic acid, 3-[4-[4-(5-chloro-2-methylphenyl)-1-piperazinyl]-1-  
 (tetrahydro-2H-pyran-2-yl)-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-,  
 1,1-dimethylethyl ester, (2E)- (CA INDEX NAME)

Double bond geometry as shown.

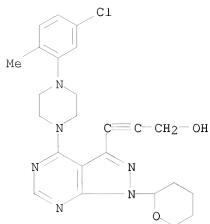




RN 871338-27-1 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[4-(5-chloro-2-methylphenyl)-1-piperazinyl]-3-[3-[[[1,1-dimethylethyl]dimethylsilyl]oxy]-1-propyn-1-yl]-1-(tetrahydro-2H-pyran-2-yl)- (CA INDEX NAME)

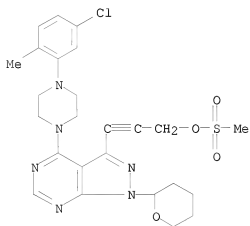


RN 871338-28-2 CAPLUS  
 CN 2-Propyn-1-ol, 3-[[4-[4-(5-chloro-2-methylphenyl)-1-piperazinyl]-1-(tetrahydro-2H-pyran-2-yl)-1H-pyrazolo[3,4-d]pyrimidin-3-yl]- (CA INDEX NAME)



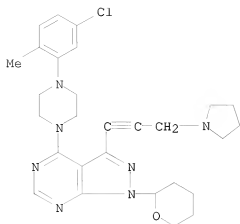
RN 871338-29-3 CAPLUS

CN 2-Propyn-1-ol, 3-[4-[4-(5-chloro-2-methylphenyl)-1-piperazinyl]-1-(tetrahydro-2H-pyran-2-yl)-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-, 1-methanesulfonate (CA INDEX NAME)



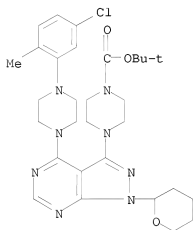
RN 871338-30-6 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[4-(5-chloro-2-methylphenyl)-1-piperazinyl]-3-[3-(1-pyrrolidinyl)-1-propyn-1-yl]-1-(tetrahydro-2H-pyran-2-yl)- (CA INDEX NAME)



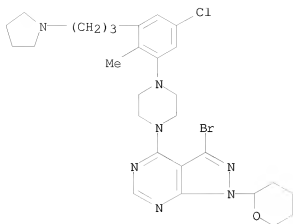
RN 871338-37-3 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[4-[4-(5-chloro-2-methylphenyl)-1-piperazinyl]-1-(tetrahydro-2H-pyran-2-yl)-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



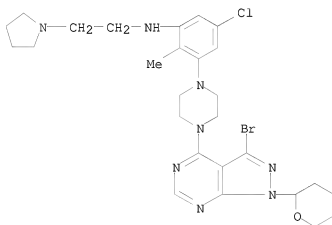
RN 871340-51-1 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 3-bromo-4-[4-[5-chloro-2-methyl-3-[3-(1-pyrrolidinyl)propyl]phenyl]-1-piperazinyl]-1-(tetrahydro-2H-pyran-2-yl)- (CA INDEX NAME)



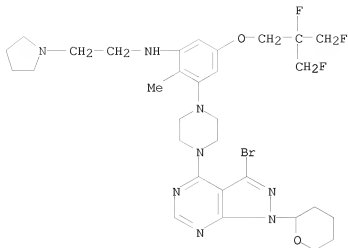
RN 871340-77-1 CAPLUS

CN 1-Pyrrolidineethanamine, N-[3-[4-[3-bromo-1-(tetrahydro-2H-pyran-2-yl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]-1-piperazinyl]-5-chloro-2-methylphenyl]- (CA INDEX NAME)



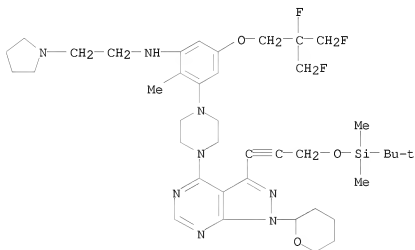
RN 871341-92-3 CAPLUS

CN 1-Pyrrolidineethanamine, N-[3-[4-[3-bromo-1-(tetrahydro-2H-pyran-2-yl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]-1-piperazinyl]-5-[2,3-difluoro-2-(fluoromethyl)propoxy]-2-methylphenyl]- (CA INDEX NAME)



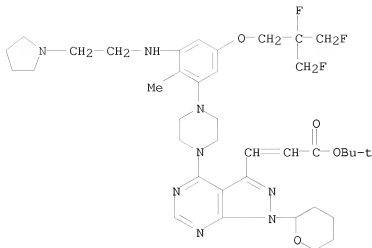
RN 871341-93-4 CAPLUS

CN 1-Pyrrolidineethanamine, N-[5-[2,3-difluoro-2-(fluoromethyl)propoxy]-3-[[4-[[3-[3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1-propyn-1-yl]-1-(tetrahydro-2H-pyran-2-yl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]-1-piperazinyl]-2-methylphenyl]- (CA INDEX NAME)

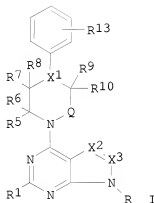


RN 871341-95-6 CAPLUS

CN 2-Propenoic acid, 3-[4-[4-[5-[2,3-difluoro-2-(fluoromethyl)propoxy]-2-methyl-3-[[[2-(1-pyrrolidinyl)ethyl]amino]phenyl]-1-piperazinyl]-1-(tetrahydro-2H-pyran-2-yl)-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



GI



AB Pyrazolo-pyrimidine derivs. I, wherein X1 is N, CR2. X2 is N, CR3; X3 is N, CR4, but when X2 is N then X3 is CR4; R is H, halogen, tri-halomethyl, substituted nitrogen, substituted sulfur, sulfonyl, sulfonamide, carboxylate, amide, substituted oxygen, acyl, alkyl, aryl, heterocycle, heterocycloalkyl, arylalkyl R1-R13 are independently H, halogen, tri-halomethyl, CN, NO2, substituted nitrogen, substituted sulfur, sulfonyl, sulfonamide, carboxylate, amide, substituted oxygen, acyl, alkyl, aryl, heterocycle, heterocycloalkyl, arylalkyl; Q is (C)nR11R12; n is 0-1 are prepared as kinase modulators. Combination chemotherapy and structure activity of title compds. are reported. The compds. modulate protein kinase enzymic activity to modulate cellular activities such as proliferation, differentiation, programmed cell death, migration and chemoinvasion. Compds. of the invention inhibit, regulate and/or modulate kinases, particularly p70S6 and/or AKT kinases. Methods of using and preparing the compds., and pharmaceutical compns. thereof, to treat kinase-dependent diseases and conditions are also an aspect of the

invention. Thus, 3-(azetidin-3-ylidene-methyl)-4-[4-(5-chloro-2-methylphenyl)piperazin-1-yl]-1H-pyrazolo[3,4-d]pyrimidine was prepared and tested in vitro as kinase modulator (IC<sub>50</sub> > 1000 nM).

L14 ANSWER 10 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:612301 CAPLUS

DOCUMENT NUMBER: 143:153230

TITLE: Preparation of substituted purines and other bicyclic heterocycles as p-38 kinase inhibitors

INVENTOR(S): Dong, Qing; Wang, Jianqiang; Lan, Jiong; Lang, Hengyuan

PATENT ASSIGNEE(S): Triad Therapeutics, Inc., USA; Novartis Pharma AG

SOURCE: PCT Int. Appl., 149 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005063766	A2	20050714	WO 2004-US43682	20041223
WO 2005063766	A3	20050909		
<p>W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LG, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW</p> <p>RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG</p>				
AU 2004309420	A1	20050714	AU 2004-309420	20041223
CA 2548326	A1	20050714	CA 2004-2548326	20041223
EP 1699800	A2	20060913	EP 2004-815697	20041223
<p>R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS</p>				
CN 1898243	A	20070117	CN 2004-80038275	20041223
BR 2004018112	A	20070417	BR 2004-18112	20041223
JP 2007517052	T	20070628	JP 2006-547489	20041223
IN 2006CN02266	A	20070608	IN 2006-CN2266	20060622
MX 2006PA07314	A	20060809	MX 2006-PA7314	20060623
US 20070142405	A1	20070621	US 2006-584076	20060823
PRIORITY APPLN. INFO.:			US 2003-532529P	P 20031223
			US 2004-575113P	P 20040528
			WO 2004-US43682	W 20041223

OTHER SOURCE(S): MARPAT 143:153230

IT 53645-78-6P 858357-97-8P 858357-98-9P

858357-99-0P 858358-00-6P 858358-01-7P

858358-02-8P 858358-03-9P 858358-04-0P

858358-05-1P 858358-06-2P

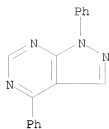
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted purines and other bicyclic heterocycles as p-38 kinase inhibitors for the treatment of inflammatory disease, autoimmune disease etc.)

RN 53645-78-6 CAPLUS

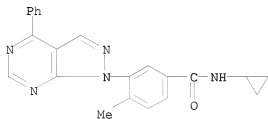
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1,4-diphenyl- (CA INDEX NAME)





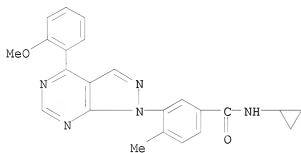
RN 858357-97-8 CAPLUS

CN Benzamide, N-cyclopropyl-4-methyl-3-(4-phenyl-1H-pyrazolo[3,4-d]pyrimidin-1-yl)- (CA INDEX NAME)



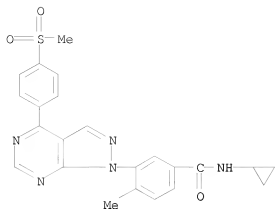
RN 858357-98-9 CAPLUS

CN Benzamide, N-cyclopropyl-3-[4-(2-methoxyphenyl)-1H-pyrazolo[3,4-d]pyrimidin-1-yl]-4-methyl- (CA INDEX NAME)



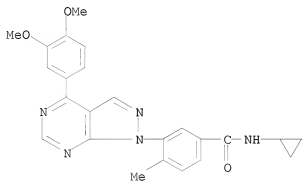
RN 858357-99-0 CAPLUS

CN Benzamide, N-cyclopropyl-4-methyl-3-[4-[4-(methanesulfonyl)phenyl]-1H-pyrazolo[3,4-d]pyrimidin-1-yl]- (CA INDEX NAME)



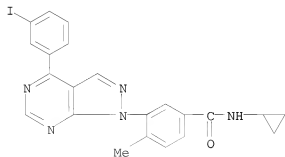
RN 858358-00-6 CAPLUS

CN Benamide, N-cyclopropyl-3-[4-(3,4-dimethoxyphenyl)-1H-pyrazolo[3,4-d]pyrimidin-1-yl]-4-methyl- (CA INDEX NAME)



RN 858358-01-7 CAPLUS

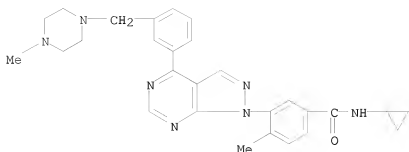
CN Benamide, N-cyclopropyl-3-[4-(3-iodophenyl)-1H-pyrazolo[3,4-d]pyrimidin-1-yl]-4-methyl- (CA INDEX NAME)



RN 858358-02-8 CAPLUS

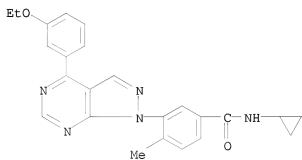
CN Benamide, N-cyclopropyl-4-methyl-3-[4-[3-[(4-methyl-1-piperazinyl)methyl]phenyl]-1H-pyrazolo[3,4-d]pyrimidin-1-yl]- (CA INDEX NAME)

NAME)



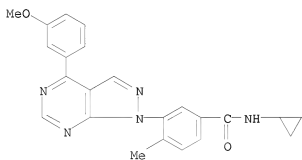
RN 858358-03-9 CAPLUS

CN Benzamide, N-cyclopropyl-3-[4-(3-ethoxyphenyl)-1H-pyrazolo[3,4-d]pyrimidin-1-yl]-4-methyl- (CA INDEX NAME)



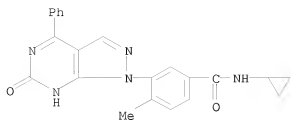
RN 858358-04-0 CAPLUS

CN Benzamide, N-cyclopropyl-3-[4-(3-methoxyphenyl)-1H-pyrazolo[3,4-d]pyrimidin-1-yl]-4-methyl- (CA INDEX NAME)



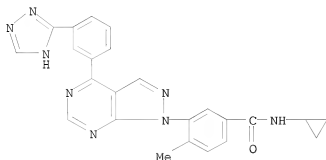
RN 858358-05-1 CAPLUS

CN Benzamide, N-cyclopropyl-3-(5,6-dihydro-6-oxo-4-phenyl-1H-pyrazolo[3,4-d]pyrimidin-1-yl)-4-methyl- (CA INDEX NAME)

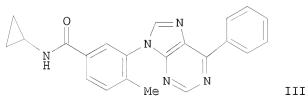
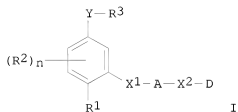


RN 858358-06-2 CAPLUS

CN Benamide, N-cyclopropyl-4-methyl-3-[4-[3-(1H-1,2,4-triazol-5-yl)phenyl]-1H-pyrazolo[3,4-d]pyrimidin-1-yl]- (CA INDEX NAME)



GI



AB The present invention discloses preparation of bicyclic heterocyclic compds., such as I [R1 = halo, alkyl, cycloalkyl, alkynyl, haloalkyl, alkoxy, haloalkoxy, NR4R5, OR4; R2 = alkyl, cycloalkyl, halo, trifluoromethyl, trifluoromethoxy, CN, NR4R5, OR4, etc.; R3 = H, alkyl, cycloalkyl, OR4, heteroaryl, heterocycle; R4, R5 = H, alkyl, cycloalkyl; n = 0-2; Y = C(:O)NH, NHC(:O), NHC(:O)NH, SO2NH, NHSO2, CO; X1 = single bond, alkylene,

O, S, SO<sub>2</sub>, CO, CONH; A = bicyclic heterocycle; X<sub>2</sub> = single bond, alkylene, O, S, NH, alkylamino, SO<sub>2</sub>, CO, CONH; D = monocyclic or bicyclic aromatic or nonarom. ring containing up to four heteroatoms], or a pharmaceutically acceptable derivs. thereof, for their therapeutic use as p38 kinase, including p38 $\alpha$  and p38 $\beta$  kinase, inhibitors. Thus, N-cyclopropyl-3-hydrazino-4-methyl-benzamide (also prepared) was reacted with aminomalononitrile p-toluene sulfonate to afford 3-(5-amino-4-cyanoimidazol-1-yl)-N-cyclopropyl-4-methyl-benzamide, which on reaction with phenylmagnesium bromide, provided 3-(5-amino-4-benzoyl-imidazol-1-yl)-N-cyclopropyl-4-methyl-benzamide (II). A mixture of benzamide derivative II, formamide and acetic acid was heated in the microwave to afford purine derivative III. Pharmaceutical compns. containing I are also provided.

#### Methods

of treatment, prevention or amelioration of one or more symptoms of p38 kinase mediated diseases and disorders, including, but not limited to, inflammatory diseases and disorders are also provided.

L14 ANSWER 11 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:216604 CAPLUS

DOCUMENT NUMBER: 142:291339

TITLE: Compositions and methods using small mol. Trp-p8 modulators for the treatment of diseases associated with Trp-p8 expression

INVENTOR(S): Natarajan, Sateesh K.; Moreno, Ofir; Graddis, Thomas J.; Duncan, David; Laus, Reiner; Chen, Feng

PATENT ASSIGNEE(S): Dendreon Corporation, USA

SOURCE: PCT Int. Appl., 120 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005020897	A2	20050310	WO 2004-US26931	20040820
WO 2005020897	A3	20050811		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2535265	A1	20050310	CA 2004-2535265	20040820
US 20050054651	A1	20050310	US 2004-923413	20040820
EP 1663962	A2	20060607	EP 2004-781589	20040820
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK			
JP 2007503392	T	20070222	JP 2006-524040	20040820
PRIORITY APPLN. INFO.:			US 2003-497384P	P 20030822
			WO 2004-US26931	W 20040820

OTHER SOURCE(S): MARPAT 142:291339

IT 305337-69-3

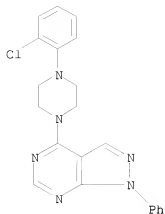
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL

(Biological study); USES (Uses)

(small mol. Trp-p8 modulators for treatment of diseases associated with Trp-p8 expression)

RN 305337-69-3 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[4-(2-chlorophenyl)-1-piperazinyl]-1-phenyl- (CA INDEX NAME)



AB Provided are small-mol. Trp-p8 modulators, including Trp-p8 agonists and Trp-p8 antagonists, and compns. comprising small-mol. Trp-p8 agonists as well as methods for identifying and characterizing small-mol. Trp-p8 modulators and methods for decreasing viability and/or inhibiting growth of Trp-p8 expressing cells, methods for activating Trp-p8-mediated cation influx, methods for stimulating apoptosis and/or necrosis, and related methods for the treatment of diseases, including cancers such as lung, breast, colon, and/or prostate cancers as well as other diseases, such as benign prostatic hyperplasia, that are associated with Trp-p8 expression. Preparation of selected p-menthane derivs. is described.

L14 ANSWER 12 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2004:857167 CAPLUS  
 DOCUMENT NUMBER: 141:350186  
 TITLE: Preparation of pyrazolopyrimidines as anti-enterovirus compounds  
 INVENTOR(S): Chern, Jyh-haur; Shia, Kak-shan; Shih, Shin-ru; Hsu, Tsu-an; Tai, Chia-liang  
 PATENT ASSIGNEE(S): Taiwan  
 SOURCE: U.S. Pat. Appl. Publ., 17 pp.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20040204400	A1	20041014	US 2003-444747	20030523
US 6815444	B2	20041109		
TW 259083	B	20060801	TW 2003-92114063	20030523
			US 2002-382925P	P 20020524

PRIORITY APPLN. INFO.:

OTHER SOURCE(S): MARPAT 141:350186

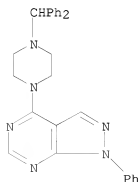
IT 300570-16-5P 305337-64-8P 313518-82-0P  
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 717098-85-6P 717098-86-7P 717098-91-4P  
 717098-92-5P 717098-93-6P 717098-94-7P  
 717098-95-8P 717098-96-9P 717098-97-0P  
 775343-76-5P 775343-77-6P 775343-78-7P  
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 775343-97-0P 775343-98-1P 775343-99-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)

(preparation of pyrazolopyrimidines as anti-enterovirus compds.)

RN 300570-16-5 CAPLUS

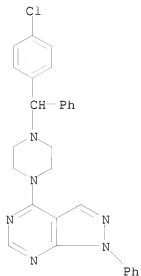
CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[4-(diphenylmethyl)-1-piperazinyl]-1-phenyl- (CA INDEX NAME)





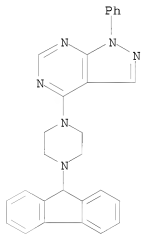
RN 305337-64-8 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[4-[(4-chlorophenyl)phenylmethyl]-1-piperazinyl]-1-phenyl- (CA INDEX NAME)



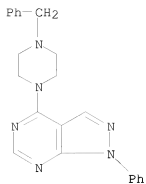
RN 313518-82-0 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[4-(9H-fluoren-9-yl)-1-piperazinyl]-1-phenyl- (CA INDEX NAME)



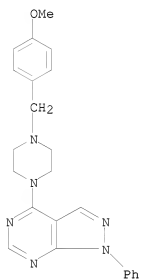
RN 314034-41-8 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-phenyl-4-[4-(phenylmethyl)-1-piperazinyl]- (CA INDEX NAME)



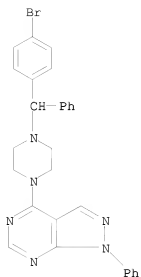
RN 612038-02-5 CAPLUS

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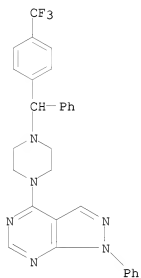
RN 717098-81-2 CAPLUS

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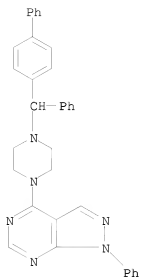
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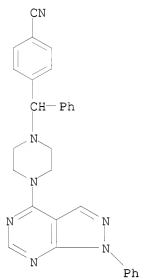


RN 717098-83-4 CAPLUS

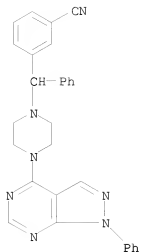
CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[4-([1,1'-biphenyl]-4-ylphenylmethyl)-1-piperazinyl]-1-phenyl- (CA INDEX NAME)



RN 717098-84-5 CAPLUS  
 CN Benzonitrile, 4-[phenyl[4-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-1-piperazinyl]methyl]- (CA INDEX NAME)

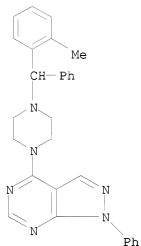


RN 717098-85-6 CAPLUS  
 CN Benzonitrile, 3-[phenyl[4-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-1-piperazinyl]methyl]- (CA INDEX NAME)



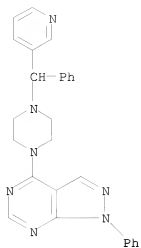
RN 717098-86-7 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[4-[(2-methylphenyl)phenylmethyl]-1-piperazinyl]-1-phenyl- (CA INDEX NAME)



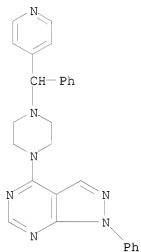
RN 717098-91-4 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-phenyl-4-[4-(phenyl-3-pyridinylmethyl)-1-piperazinyl]- (CA INDEX NAME)



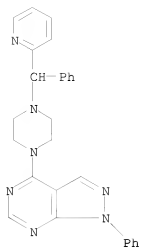
RN 717098-92-5 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-phenyl-4-[4-(phenyl-4-pyridinylmethyl)-1-piperazinyl]- (CA INDEX NAME)



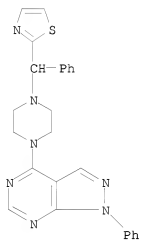
RN 717098-93-6 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-phenyl-4-[4-(phenyl-2-pyridinylmethyl)-1-piperazinyl]- (CA INDEX NAME)



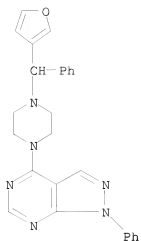
RN 717098-94-7 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-phenyl-4-[4-(phenyl-2-thiazolylmethyl)-1-piperazinyl]- (CA INDEX NAME)



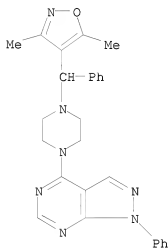
RN 717098-95-8 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[4-(3-furanylphenylmethyl)-1-piperazinyl]-1-phenyl- (CA INDEX NAME)



RN 717098-96-9 CAPLUS

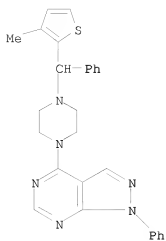
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RN 717098-97-0 CAPLUS

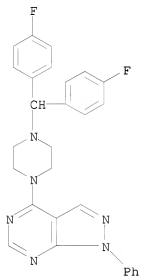
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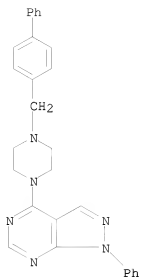
RN 775343-76-5 CAPLUS

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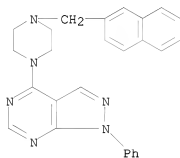


RN 775343-77-6 CAPLUS

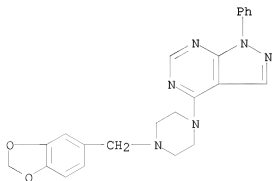
CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[4-([1,1'-biphenyl]-4-ylmethyl)-1-piperazinyl]-1-phenyl- (CA INDEX NAME)



RN 775343-78-7 CAPLUS  
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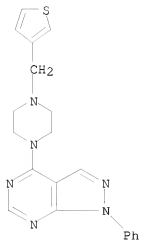


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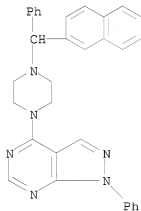
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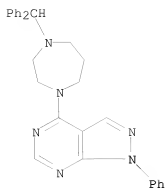
RN 775343-81-2 CAPLUS

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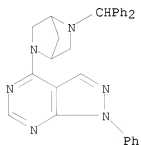
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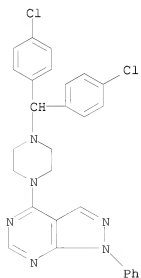
RN 775343-83-4 CAPLUS

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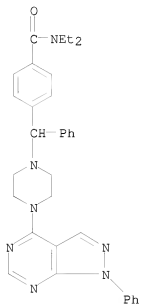
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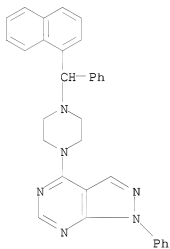
RN 775343-85-6 CAPLUS

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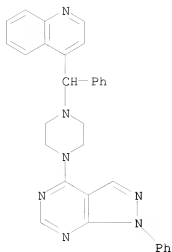
RN 775343-86-7 CAPLUS

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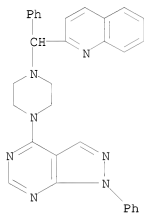
RN 775343-87-8 CAPLUS

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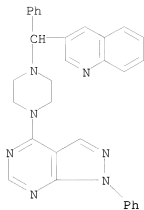
RN 775343-88-9 CAPLUS

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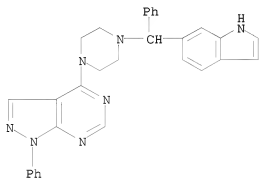
RN 775343-89-0 CAPLUS

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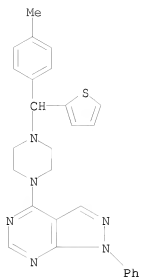
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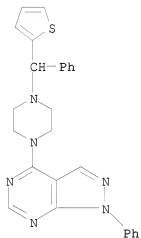
RN 775343-91-4 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[4-[(4-methylphenyl)-2-thienylmethyl]-1-piperazinyl]-1-phenyl- (CA INDEX NAME)



RN 775343-92-5 CAPLUS

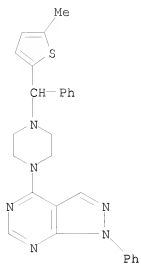
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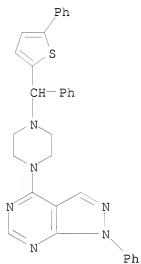
CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[4-[(5-methyl-2-thienyl)phenylmethyl]-1-piperazinyl]-1-phenyl- (CA INDEX NAME)





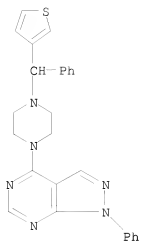
RN 775343-94-7 CAPLUS

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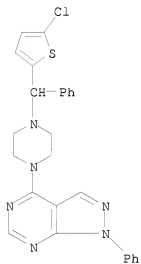
RN 775343-95-8 CAPLUS

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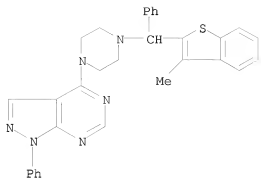
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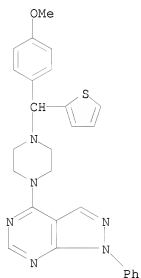
RN 775343-97-0 CAPLUS

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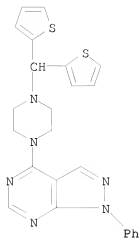
RN 775343-98-1 CAPLUS

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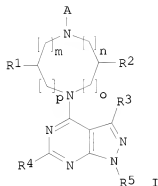


RN 775343-99-2 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[4-(di-2-thienylmethyl)-1-piperazinyl]-1-phenyl- (CA INDEX NAME)



GI



AB The title compds. [I; A = (CH<sub>2</sub>)<sub>q</sub>CHRaRb; R<sub>1</sub>, R<sub>2</sub> = H, halo, CN, NO<sub>2</sub>, alkyl; or R<sub>1</sub> and R<sub>2</sub> taken together is (CH<sub>2</sub>)<sub>r</sub>; R<sub>3</sub>, R<sub>4</sub> = H, halo, CN, NO<sub>2</sub>, alkyl; R<sub>5</sub>, Ra, Rb = (un)substituted aryl, aralkyl, heteroaryl; m, n, o, p, r = 0 or 1; q = 0-2; provided that the sum of m, n, o, and p = 1, 2, 3, or 4], were prepared. Thus, reacting 4-chloro-1-phenyl-1H-pyrazolo[3,4-d]pyrimidine with 1-(diphenylmethyl)piperazine afforded 95% 4-(4-benzhydrylpiperazino)-1-phenyl-1H-pyrazolo[3,4-d]pyrimidine. The 5 of 42 prepared compds. I were tested against enteroviruses and non-. All 5 pyrazolopyrimidine compds. showed antiviral activity against all enteroviruses tested (IC<sub>50</sub> values less than 1 μM and as low as 0.085 μM). In particular, against COX-A24, -B2, -B3, or -B4. In contrast, these compds. showed little efficacy against the non-enteroviruses (Ic<sub>50</sub> values higher than 25 μM).

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 13 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:368857 CAPLUS

DOCUMENT NUMBER: 140:386000

TITLE: Compounds, compositions and methods for modulating fat metabolism for treatment of metabolic disorders

INVENTOR(S): Gaudriault, Georges; Kilinc, Ahmet; Bousquet, Olivier; Goupil-Lamy, Anne; Harosh, Itzik

PATENT ASSIGNEE(S): Obetherapy Biotechnology, Fr.

SOURCE: PCT Int. Appl., 461 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004037159	A2	20040506	WO 2003-IL860	20031023
WO 2004037159	A3	20040715		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2003274652	A1	20040513	AU 2003-274652	20031023
PRIORITY APPLN. INFO.:			US 2002-420316P	P 20021023
			WO 2003-IL860	W 20031023

OTHER SOURCE(S): MARPAT 140:386000

IT 393822-08-7 393822-71-4 393823-03-5

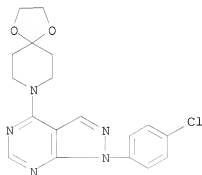
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL

(Biological study); USES (Uses)

(comps., compns. and methods for modulating fat metabolism for treatment of metabolic disorders)

RN 393822-08-7 CAPLUS

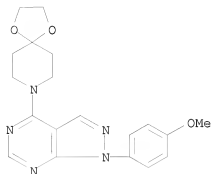
CN 1,4-Dioxo-8-azaspiro[4.5]decane, 8-[1-(4-chlorophenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]- (CA INDEX NAME)



RN 393822-71-4 CAPLUS

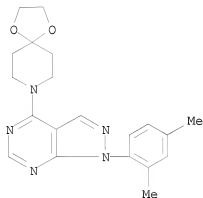
CN 1,4-Dioxo-8-azaspiro[4.5]decane, 8-[1-(4-methoxyphenyl)-1H-pyrazolo[3,4-

d]pyrimidin-4-yl]- (CA INDEX NAME)



RN 393823-03-5 CAPLUS

CN 1,4-Dioxo-8-azaspiro[4.5]decane, 8-[1-(2,4-dimethylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]- (CA INDEX NAME)



AB Methods and compns. of identifying candidate compds., for modulating fat metabolism and/or inhibiting Apobec-1 activity are provided. The invention relates to compds. and pharmaceutical compns. which are useful for regulating fat metabolism and can be used for treatment of diseases and disorders selected from the group consisting of overweight, obesity, atherosclerosis, hypertension, non-insulin dependent diabetes mellitus, pancreatitis, hypercholesteremia, hypertriglyceridemia, hyperlipidemia.

L14 ANSWER 14 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:346253 CAPLUS

DOCUMENT NUMBER: 141:89059

TITLE: Design, synthesis, and structure-activity relationships of pyrazolo[3,4-d]pyrimidines: a novel class of potent enterovirus inhibitors

AUTHOR(S): Chern, Jyh-Haur; Shia, Kak-Shan; Hsu, Tsu-An; Tai, Chia-Liang; Lee, Chung-Chi; Lee, Yen-Chun; Chang, Chih-Shiang; Tseng, Sung-Nien; Shih, Shin-Ru  
CORPORATE SOURCE: Division of Biotechnology and Pharmaceutical Research, National Health Research Institutes, Taipei, Taiwan, 114, Peop. Rep. China

SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(10), 2519-2525

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

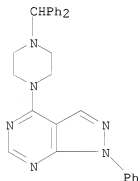
LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:89059

IT 300570-16-5P, 4-[4-(Diphenylmethyl)-1-piperazinyl]-1-phenyl-1H-pyrazolo[3,4-d]pyrimidine 305337-64-8P, 4-[4-[(4-Chlorophenyl)phenylmethyl]-1-piperazinyl]-1-phenyl-1H-pyrazolo[3,4-d]pyrimidine 717098-81-2P 717098-82-3P 717098-83-4P 717098-84-5P 717098-85-6P 717098-86-7P 717098-91-4P 717098-92-5P 717098-93-6P 717098-94-7P 717098-95-8P 717098-96-9P 717098-97-0P 717098-98-1P 717098-99-2P 717099-00-8P 717099-01-9P  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
(preparation of pyrazolo[3,4-d]pyrimidine derivs. and study of their activity as inhibitors of human enterovirus, coxsackievirus, echovirus, influenza virus, herpes simplex virus and rhinovirus)

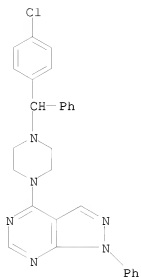
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CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[4-(diphenylmethyl)-1-piperazinyl]-1-phenyl- (CA INDEX NAME)



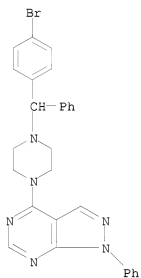
RN 305337-64-8 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[4-[(4-chlorophenyl)phenylmethyl]-1-piperazinyl]-1-phenyl- (CA INDEX NAME)



RN 717098-81-2 CAPLUS

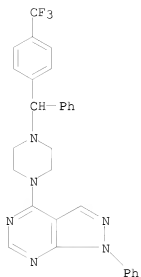
CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[4-[(4-bromophenyl)phenylmethyl]-1-piperazinyl]-1-phenyl- (CA INDEX NAME)



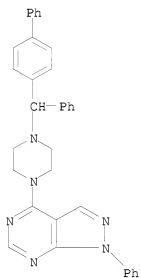
RN 717098-82-3 CAPLUS

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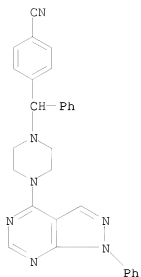




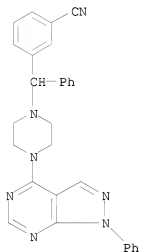
RN 717098-83-4 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[4-([1,1'-biphenyl]-4-yl)phenylmethyl]-1-piperazinyl-1-phenyl- (CA INDEX NAME)



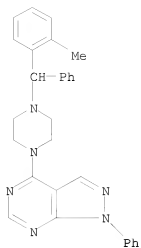
RN 717098-84-5 CAPLUS  
 CN Benzonitrile, 4-[phenyl[4-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-1-piperazinyl]methyl]- (CA INDEX NAME)



RN 717098-85-6 CAPLUS  
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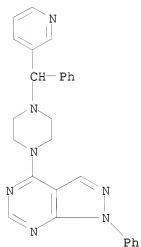


RN 717098-86-7 CAPLUS  
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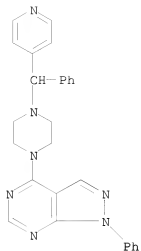
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CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-phenyl-4-[4-(phenyl-3-pyridinylmethyl)-1-piperazinyl]- (CA INDEX NAME)



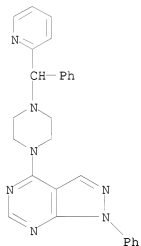
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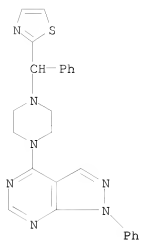
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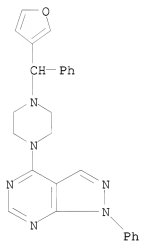
RN 717098-94-7 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-phenyl-4-[4-(phenyl-2-thiazolylmethyl)-1-piperazinyl]- (CA INDEX NAME)



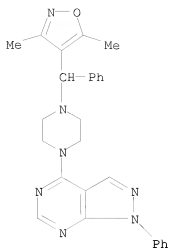
RN 717098-95-8 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[4-(3-furanylphenylmethyl)-1-piperazinyl]-1-phenyl- (CA INDEX NAME)



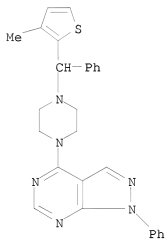
RN 717098-96-9 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[4-[(3,5-dimethyl-4-isoxazolyl)phenylmethyl]-1-piperazinyl]-1-phenyl- (CA INDEX NAME)



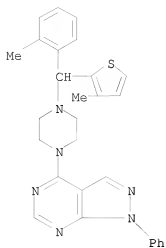
RN 717098-97-0 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[4-[(3-methyl-2-thienyl)phenylmethyl]-1-piperazinyl]-1-phenyl- (CA INDEX NAME)



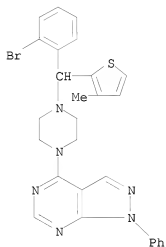
RN 717098-98-1 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[4-[(2-methylphenyl)(3-methyl-2-thienyl)methyl]-1-piperazinyl]-1-phenyl- (CA INDEX NAME)



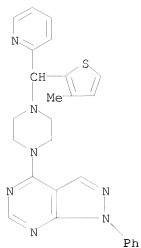
RN 717098-99-2 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[4-[(2-bromophenyl)(3-methyl-2-thienyl)methyl]-1-piperazinyl]-1-phenyl- (CA INDEX NAME)



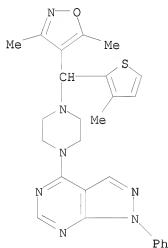
RN 717099-00-8 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[4-[(3-methyl-2-thienyl)-2-pyridinylmethyl]-1-piperazinyl]-1-phenyl- (CA INDEX NAME)

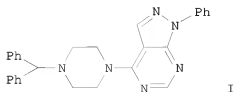


RN 717099-01-9 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[4-((3,5-dimethyl-4-isoxazolyl)(3-methyl-2-thienyl)methyl)-1-piperazinyl]-1-phenyl- (CA INDEX NAME)



GI



I

AB A series of pyrazolo[3,4-d]pyrimidines was synthesized and their antiviral

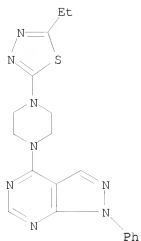


activity was evaluated in a plaque reduction assay. It is very interesting that this class of compds. provide remarkable evidence that they are very specific for human enteroviruses, in particular, coxsackieviruses. Some derivs. proved to be highly effective in inhibiting enterovirus replication at nanomolar concns. SAR studies revealed that the Ph group at the N-1 position and the hydrophobic diarylmethyl group at the piperazine largely influenced the in vitro antienteroviral activity of this new class of potent antiviral agents. It was found that (thienyl)pyrazolo[3,4-d]pyrimidine derivs. in general exhibited high activity against coxsackievirus B3 (IC<sub>50</sub> = 0.063-0.089  $\mu$ M) and moderate activity against enterovirus 71 (IC<sub>50</sub> = 0.32-0.65  $\mu$ M) with no apparent cytotoxic effect toward RD (rhabdomyosarcoma) cell lines (CC<sub>50</sub>>25  $\mu$ M). Thus, 4-[4-(diphenylmethyl)-1-piperazinyl]-1-phenyl-1H-pyrazolo[3,4-d]pyrimidine (I) was found to possess significant antienteroviral activity.

REFERENCE COUNT: 18      THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 15 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2004:331897 CAPLUS  
 DOCUMENT NUMBER: 140:350578  
 TITLE: Small organic compounds for modulation of cholesterol transport via regulation of the scavenger receptor SR-BI for HDL  
 INVENTOR(S): Nieland, Thomas J. F.; Krieger, Monty; Kirchhausen, Tomas  
 PATENT ASSIGNEE(S): Massachusetts Institute of Technology, USA; Center for Blood Research, Inc.  
 SOURCE: PCT Int. Appl., 51 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004032716	A2	20040422	WO 2003-US31918	20031008
WO 2004032716	A9	20040819		
WO 2004032716	A3	20040930		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2501685	A1	20040422	CA 2003-2501685	20031008
AU 2003288925	A1	20040504	AU 2003-288925	20031008
US 20040171073	A1	20040902	US 2003-681746	20031008
EP 1562605	A2	20050817	EP 2003-781314	20031008
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
JP 2006515274	T	20060525	JP 2004-543548	20031008
PRIORITY APPLN. INFO.:			US 2002-417083P	P 20021008
			WO 2003-US31918	W 20031008
IT 313364-25-9				
RL:	PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)			
	(small organic compds. for modulation of cholesterol transport via regulation of the scavenger receptor SR-BI for HDL)			
RN 313364-25-9	CAPLUS			
CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[4-(5-ethyl-1,3,4-thiadiazol-2-yl)-1-piperazinyl]-1-phenyl-	(CA INDEX NAME)			



AB Methods for regulation of lipid and cholesterol uptake are described which are based on regulation of the expression or function of the SR-BI HDL receptor. The examples demonstrate that estrogen dramatically down-regulates SR-BI under conditions of tremendous upregulation of the LDL-receptor. The examples also demonstrate the upregulation of SR-BI in rat adrenal membranes and other non-placental steroidogenic tissues from animals treated with estrogen, but not in other non-placental non-steroidogenic tissues, including lung, liver, and skin. Examples further demonstrate the uptake of fluorescently labeled HDL into the liver cells of animal, which does not occur when the animals are treated with estrogen. Examples also demonstrate the *in vivo* effects of SR-BI expression on HDL metabolism, in mice transiently overexpressing hepatic SR-BI following recombinant adenovirus infection. Overexpression of the SR-BI in the hepatic tissue caused a dramatic decrease in cholesterol blood levels. These results demonstrate that modulation of SR-BI levels, either directly or indirectly, can be used to modulate levels of cholesterol in the blood. Over 200 small organic compds. are identified that alter the transfer of lipids between HDL and cells mediated by the HDL receptor SR-BI, cellular and selective lipid uptake of HDL cholesteryl ether, and efflux of cellular cholesterol to HDL; several compds. have IC50 values in the micromolar or lower range. They specifically alter SR-BI binding, as they required the expression of active SR-BI receptors and they did not interfere with several clathrin-dependent and independent endocytic pathways, the secretory pathway, nor the actin- or tubulin cytoskeletal networks. Strikingly, inhibition of lipid transfer was accompanied by enhanced HDL binding affinity (reduced dissociation rates).

L14 ANSWER 16 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:307614 CAPLUS  
DOCUMENT NUMBER: 140:332509  
TITLE: Pharmaceutical compositions containing  
spiroisoquinolines as small-conductance  
calcium-activated potassium channel (SK channel)  
blockers and acetylcholine esterase inhibitors  
INVENTOR(S): Takamuro, Iwao; Honma, Koichi; Ishida, Akihiko;  
Taniguchi, Hiroyuki; Onoda, Yuichi  
PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 334 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004115450	A	20040415	JP 2002-282311	20020927
PRIORITY APPLN. INFO.:			JP 2002-282311	20020927

OTHER SOURCE(S): MARPAT 140:332509

IT 470428-98-9P 470429-07-3P 470430-40-1P  
470430-49-0P 470432-18-9P 470432-22-5P  
470432-36-1P 470432-93-0P 470433-01-3P  
470438-23-4P 470438-32-5P

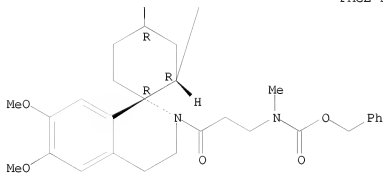
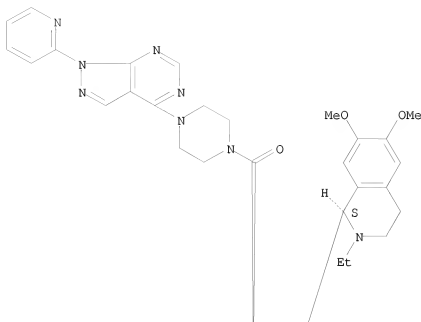
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)

(preparation of spiroisoquinolines as small-conductance Ca<sup>2+</sup>-activated K<sup>+</sup>  
channel blockers and acetylcholine esterase inhibitors for treatment of  
diseases)

RN 470428-98-9 CAPLUS

CN Carbamic acid, [3-[(1R,2R,4R)-2-[(1S)-2-ethyl-1,2,3,4-tetrahydro-6,7-  
dimethoxy-1-isoquinoliny]-3',4'-dihydro-6',7'-dimethoxy-4-[[4-[1-(2-  
pyridinyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]-1-  
piperazinyl]carbonyl]spiro[cyclohexane-1,1'(2'H)-isoquinolin]-2'-yl]-3-  
oxopropyl)methyl-, phenylmethyl ester, rel- (9CI) (CA INDEX NAME)

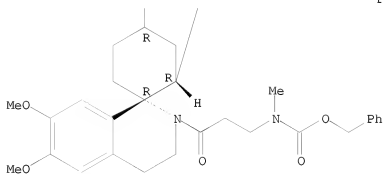
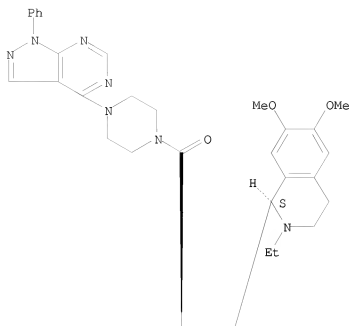
Relative stereochemistry.



RN 470429-07-3 CAPLUS

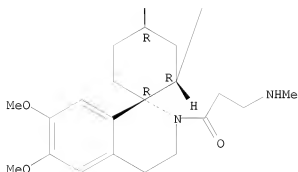
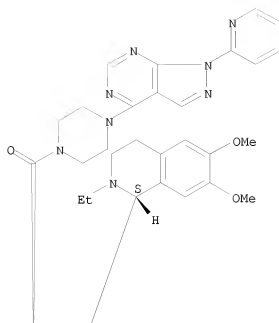
CN Carbamic acid, [3-[(1R,2R,4R)-2-[(1S)-2-ethyl-1,2,3,4-tetrahydro-6,7-dimethoxy-1-isoquinolinyl]-3',4'-dihydro-6',7'-dimethoxy-4-[[4-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-1-piperazinyl]carbonyl]spiro[cyclohexane-1,1'-(2'H)-isoquinolin]-2'-yl]-3-oxopropyl]methyl-, phenylmethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



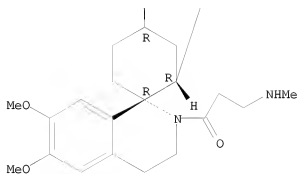
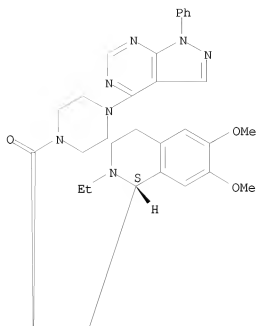
RN 470430-40-1 CAPLUS  
 CN Spiro[cyclohexane-1,1'-(2'H)-isoquinoline], 2-[(1R)-2-ethyl-1,2,3,4-tetrahydro-6,7-dimethoxy-1-isoquinolinyl]-3',4'-dihydro-6',7'-dimethoxy-2'-[3-(methylamino)-1-oxopropyl]-4-[[4-[1-(2-pyridinyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]-1-piperazinyl]carbonyl]-, (1S,2S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 470430-49-0 CAPLUS  
 CN Spiro[cyclohexane-1,1'-(2'H)-isoquinoline], 2-[(1R)-2-ethyl-1,2,3,4-tetrahydro-6,7-dimethoxy-1-isoquinolinyl]-3',4'-dihydro-6',7'-dimethoxy-2'-[3-(methylamino)-1-oxopropyl]-4-[[4-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-1-piperazinyl]carbonyl]-, (1S,2S,4S)-rel- (9CI) (CA INDEX NAME)

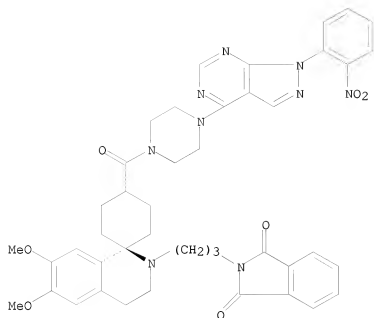
Relative stereochemistry.



RN 470432-18-9 CAPLUS  
 CN Piperazine, 1-[trans-2'-[3-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)propyl]-3',4'-dihydro-6',7'-dimethoxyspiro[cyclohexane-1,1'(2'H)-isoquinolin]-4-yl]carbonyl]-4-[1-(2-nitrophenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

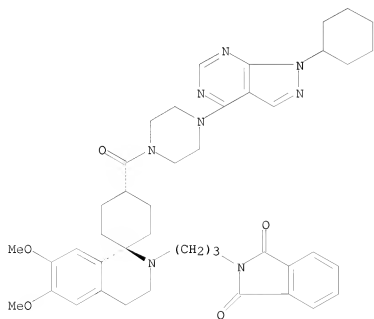




RN 470432-22-5 CAPLUS

CN Piperazine, 1-[(1-cyclohexyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-4-[[trans-2'-[3-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)propyl]-3',4'-dihydro-6',7'-dimethoxyspiro[cyclohexane-1,1'-(2'H)-isoquinolin]-4-yl]carbonyl]- (9CI)  
(CA INDEX NAME)

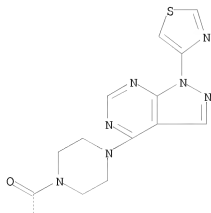
Relative stereochemistry.



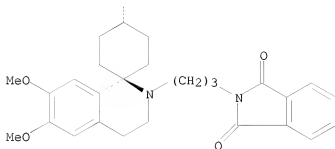
RN 470432-36-1 CAPLUS  
 CN Piperazine, 1-[[trans-2'-[3-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)propyl]-3',4'-dihydro-6',7'-dimethoxyspiro[cyclohexane-1,1'(2'H)-isoquinolin]-4-yl]carbonyl]-4-[1-(4-thiazolyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 2-A

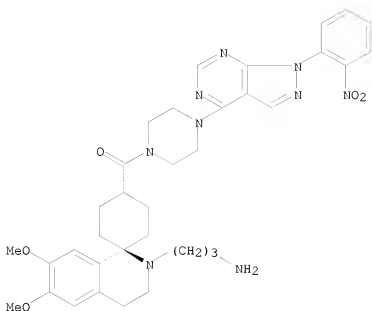


RN 470432-93-0 CAPLUS  
 CN Piperazine, 1-[[trans-2'-[(3-aminopropyl)-3',4'-dihydro-6',7'-dimethoxyspiro[cyclohexane-1,1'(2'H)-isoquinolin]-4-yl]carbonyl]-4-[1-(2-nitrophenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 470432-92-9  
CMF C35 H43 N9 O5

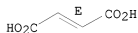
Relative stereochemistry.



CM 2

CRN 110-17-8  
CMF C4 H4 O4

Double bond geometry as shown.

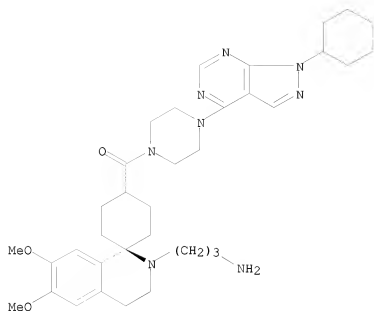


RN 470433-01-3 CAPLUS  
CN Piperazine, 1-[[trans-2'-(3-aminopropyl)-3',4'-dihydro-6',7'-dimethoxyspiro[cyclohexane-1,1'-(2'H)-isoquinolin]-4-yl]carbonyl]-4-(1-cyclohexyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 470433-00-2  
CMF C35 H50 N8 O3

Relative stereochemistry.



CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



RN 470438-23-4 CAPLUS

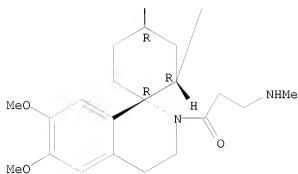
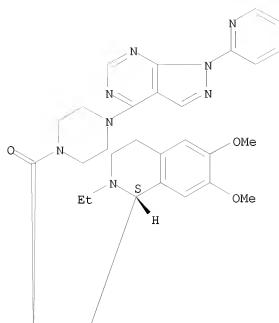
CN Spiro[cyclohexane-1,1'-(2'H)-isoquinoline], 2-[(1R)-2-ethyl-1,2,3,4-tetrahydro-6,7-dimethoxy-1-isoquinolinyl]-3',4'-dihydro-6',7'-dimethoxy-2'-[3-(methylamino)-1-oxopropyl]-4-[[4-[1-(2-pyridinyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]-1-piperazinyl]carbonyl]-, (1S,2S,4S)-rel-, (2E)-2-butenedioate (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 470430-40-1

CMF C48 H60 N10 O6

Relative stereochemistry.



CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



RN 470438-32-5 CAPLUS

CN Spiro[cyclohexane-1,1'(2'H)-isoquinoline], 2-[(1R)-2-ethyl-1,2,3,4-

tetrahydro-6,7-dimethoxy-1-isoquinolinyl]-3',4'-dihydro-6',7'-dimethoxy-2'-  
[3-(methylamino)-1-oxopropyl]-4-[[4-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-  
4-yl)-1-piperazinyl]carbonyl]-, (1S,2S,4S)-rel-, (2E)-2-butenedioate (1:2)  
(9CI) (CA INDEX NAME)

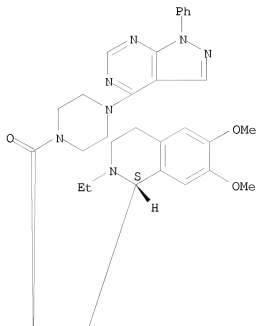
CM 1

CRN 470430-49-0

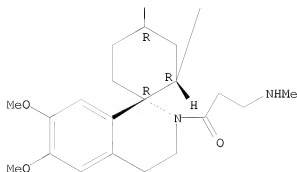
CMF C49 H61 N9 O6

Relative stereochemistry.

PAGE 1-A



PAGE 2-A



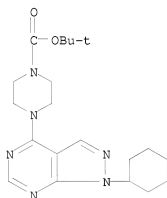
CM 2

CRN 110-17-8  
CMF C4 H4 O4

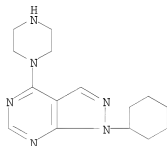
Double bond geometry as shown.



IT 470442-31-0P 470442-42-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation of spiroisoquinolines as small-conductance  $\text{Ca}^{2+}$ -activated  $\text{K}^{+}$   
channel blockers and acetylcholine esterase inhibitors for treatment of  
diseases)  
RN 470442-31-0 CAPLUS  
CN 1-Piperazinecarboxylic acid, 4-(1-cyclohexyl-1H-pyrazolo[3,4-d]pyrimidin-4-  
yl)-, 1,1-dimethylethyl ester (CA INDEX NAME)

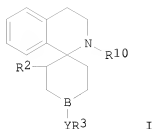


RN 470442-42-3 CAPLUS  
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-cyclohexyl-4-(1-piperazinyl)-,  
dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

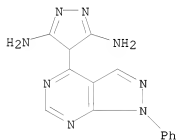
GI



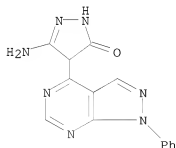
AB Title compns., useful for treatment of digestive tract function failure, central nervous disorders, myotonic dystrophy, etc., contain spiroisoquinolines I [ring A may be substituted; R10 = H, ZR1; R1 = H, (un)substituted lower alkyl, (un)substituted lower alkenyl; Y, Z = CH2, CO; R2 H, (un)substituted heterocyclyl; B = N, CH; R3 = (un)substituted NH2, (un)substituted N-containing aliphatic heterocyclyl] or their pharmacol. acceptable salts as active ingredients. Thus, (1R\*,2R\*(S\*),4R\*)-2'-[3-(methylamino)propionyl]-3',4'-dihydro-6',7'-dimethoxy-2-(2-ethyl-1,2,3,4-tetrahydro-6,7-dimethoxy-1-isoquinolyl)-4-[4-[1-(4-pyridylmethyl)-1H-pyrazolol-[3,4-d]pyrimidin-4-yl]-1-piperazinyl]carbonyl-spiro[cyclohexane-1,1'(2'H)isoquinoline] difumarate inhibited binding of 125I-apamin to SK channel in guinea pigs with IC50 value of 0.05  $\mu$ M.



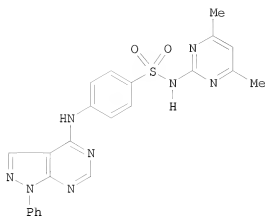
L14 ANSWER 17 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2004:65181 CAPLUS  
 DOCUMENT NUMBER: 140:287352  
 TITLE: Antimicrobial activity of amino acid, imidazole, and sulfonamide derivatives of pyrazolo[3,4-d]pyrimidine  
 AUTHOR(S): Ghorab, M. M.; Ismail, Zeinab H.; Abdel-Gawad, Soad M.; Abdel Aziem, Anhar  
 CORPORATE SOURCE: Department of Drug Radiation Research, National Centre for Radiation Research and Technology, Nasr City, Egypt  
 SOURCE: Heteroatom Chemistry (2003), Volume Date 2004, 15(1), 57-62  
 CODEN: HETCE8; ISSN: 1042-7163  
 PUBLISHER: John Wiley & Sons, Inc.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 140:287352  
 IT 675578-86-6P 675578-87-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and antimicrobial activity of amino acid, imidazole, and sulfonamide derivs. of pyrazolopyrimidine via substitution of chloropyrazolopyrimidine with amine and active methylene compds.)  
 RN 675578-86-6 CAPLUS  
 CN 4H-Pyrazole-3,5-diamine, 4-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-  
 (CA INDEX NAME)



RN 675578-87-7 CAPLUS  
 CN 3H-Pyrazol-3-one, 5-amino-2,4-dihydro-4-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)- (CA INDEX NAME)



GI



AB Derivs. of pyrazolo[3,4-d]pyrimidine with amino acid, imidazole, carbonyl, pyrazole, pyrazolone and sulfonamide moieties were synthesized. Their structure were established by elemental analyses and spectral data. Six of them were tested in vitro for antimicrobial activity. Three compds., e.g. I, were found to be almost as potent as the standard antibiotic chloramphenicol in the antibacterial test, and four compds. including I were nearly as active as terbinafine in the fungicidal test.

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2004:2886 CAPLUS

DOCUMENT NUMBER: 140:77157

TITLE: Preparation of novel purine- or pyrrolo[2,3-d]pyrimidine-2-carbonitriles for treating diseases associated with cysteine protease activity

INVENTOR(S): Bailey, Andrew; Pairaudeau, Garry; Patel, Anil; Thom, Stephen

PATENT ASSIGNEE(S): Astrazeneca AB, Swed.

SOURCE: PCT Int. Appl., 41 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004000843	A1	20031231	WO 2003-SE1079	20030623
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003243096	A1	20040106	AU 2003-243096	20030623
EP 1532148	A1	20050525	EP 2003-761002	20030623
EP 1532148	B1	20070117		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2005533804	T	20051110	JP 2004-515329	20030623
ES 2279162	T3	20070816	ES 2003-761002	20030623
US 20050203107	A1	20050915	US 2004-518815	20041220
PRIORITY APPLN. INFO.:			SE 2002-1980	A 20020624
			WO 2003-SE1079	W 20030623

OTHER SOURCE(S): MARPAT 140:77157

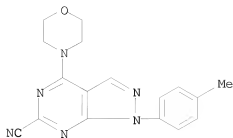
IT 640285-16-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

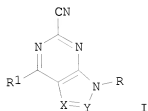
(preparation of purine- or pyrrolo[2,3-d]pyrimidine-2-carbonitriles for treating diseases associated with cysteine protease activity)

RN 640285-16-1 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine-6-carbonitrile, 1-(4-methylphenyl)-4-(4-morpholinyl)- (CA INDEX NAME)



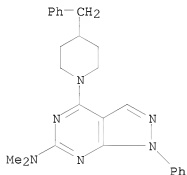
GI



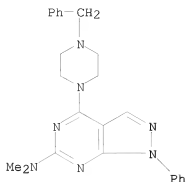
AB The title compds. [I; X = N, NH, CH, CH<sub>2</sub>; Y = N, CH, CO, CH<sub>2</sub>, CNR<sub>2</sub>R<sub>3</sub> (wherein R<sub>2</sub>, R<sub>3</sub> = H, alkyl, cycloalkyl); R = (un)substituted (hetero)aryl, H, alkyl, cycloalkyl, etc.; R<sub>1</sub> = Z(CH<sub>2</sub>)<sub>p</sub>R<sub>7</sub> (wherein p = 0-2; Z = O, NR<sub>8</sub>; R<sub>8</sub> = H, alkyl, cycloalkyl; R<sub>7</sub> = (un)substituted 5-6 membered saturated ring containing one or more O, S or N atoms, aryl or heteroaryl), NR<sub>9</sub>R<sub>10</sub> (R<sub>9</sub>, R<sub>10</sub> = H, alkyl, etc.; or NR<sub>9</sub>R<sub>10</sub> = (un)substituted 5-6 membered saturated ring optionally containing a further O, S or N atom)] which are reversible inhibitors of cysteine proteases S, K, F, L and B (no data), and therefore useful for treating diseases associated with cysteine protease activity (especially diseases associated with Cathepsin S), were prepared. Thus, a 4-step synthesis of 1-[9-(4-chlorophenyl)-2-cyano-9H-purin-6-yl]-L-prolinamide (starting from 4-chloroaniline and 5-amino-4,6-dichloro-2-propylthiopyrimidine), was given. Pharmaceutical composition comprising the compound I is claimed.

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 19 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2003:144160 CAPLUS  
 DOCUMENT NUMBER: 139:94757  
 TITLE: 6-Dimethylamino 1H-Pyrazolo[3,4-d]pyrimidine derivatives as new inhibitors of inflammatory mediators in intact cells  
 AUTHOR(S): Quintela, Jose M.; Peinador, Carlos; Gonzalez, Liliana; Devesa, Isabel; Ferrandiz, M. Luisa; Alcaraz, Maria J.; Riguera, Ricardo  
 CORPORATE SOURCE: Facultad de Ciencias, Departamento de Quimica Fundamental e Industrial, Universidad de La Coruna, La Coruna, 15071, Spain  
 SOURCE: Bioorganic & Medicinal Chemistry (2003), 11(6), 863-868  
 CODEN: BMECEP; ISSN: 0968-0896  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 139:94757  
 IT 560991-94-8P 560991-96-0P  
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and structure-activity relationship of 6-dimethylamino 1H-pyrazolo[3,4-d]pyrimidine derivs. as new inhibitors of inflammatory mediators in murine macrophages and human neutrophils)  
 RN 560991-94-8 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidin-6-amine, N,N-dimethyl-1-phenyl-4-[4-(phenylmethyl)-1-piperidinyl]- (CA INDEX NAME)



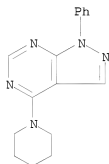
RN 560991-96-0 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidin-6-amine, N,N-dimethyl-1-phenyl-4-[4-(phenylmethyl)-1-piperazinyl]- (CA INDEX NAME)



AB The synthesis of 6-dimethylamino 1H-pyrazolo[3,4-d]pyrimidines substituted at positions 1 and 4, and their effects on murine macrophage and human neutrophil functions are described. Several of these compounds are potent inhibitors of PGE<sub>2</sub> generation in murine macrophages. This action is related to a direct effect on COX-2 activity without affecting the enzyme expression. Some of these compounds also inhibited COX-1 and COX-2 in human monocytes and showed selectivity for COX-2 inhibition.

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 20 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2003:137812 CAPLUS  
 DOCUMENT NUMBER: 139:69219  
 TITLE: The one-pot conversion of pyrimidinone derivatives to substituted pyrimidines using diphenylphosphinic chloride under mild conditions  
 AUTHOR(S): Tanji, Ken-ichi; Yokoi, Takeshi; Sugimoto, Osamu  
 CORPORATE SOURCE: Laboratory of Organic Chemistry, School of Food and Nutritional Sciences, University of Shizuoka, Shizuoka, 422-8526, Japan  
 SOURCE: Heterocycles (2003), 60(2), 413-418  
 CODEN: HTCYAM; ISSN: 0385-5414  
 PUBLISHER: Japan Institute of Heterocyclic Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 139:69219  
 IT 23000-46-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (one-pot conversion of pyrimidinones to pyrimidines using diphenylphosphinic chloride)  
 RN 23000-46-6 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-phenyl-4-(1-piperidinyl)- (CA INDEX NAME)



AB Pyrimidinone derivs. reacted with diphenylphosphinic chloride, followed by addition of nucleophiles, to afford substituted pyrimidine derivs. at a mild temperature (20-66°).  
 REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 21 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:777925 CAPLUS

DOCUMENT NUMBER: 137:294881

TITLE: A spiroisoquinoline compound, useful as an SK channel blocker and acetylcholinesterase inhibitor, for treatment of, e.g., constipation, a method for preparing the same, and an intermediate thereof

INVENTOR(S): Takamuro, Iwao; Homma, Koichi; Ishida, Akihiko; Taniguchi, Hiroyuki; Onoda, Yuichi

PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan

SOURCE: PCT Int. Appl., 464 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002079189	A2	20021010	WO 2002-JP3051	20020328
WO 2002079189	A3	20030703		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2002242996	A1	20021015	AU 2002-242996	20020328
JP 2003252871	A	20030910	JP 2002-92220	20020328
EP 1373247	A2	20040102	EP 2002-708702	20020328
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
US 20040106635	A1	20040603	US 2003-473064	20030926
PRIORITY APPLN. INFO.:			JP 2001-94710	A 20010329
			JP 2001-189010	A 20010622
			JP 2001-326866	A 20011024
			WO 2002-JP3051	W 20020328

OTHER SOURCE(S): MARPAT 137:294881

IT 470428-98-9P 470429-07-3P 470430-40-1P  
470430-49-0P 470432-18-9P 470432-22-5P  
470432-36-1P 470432-93-0P 470433-01-3P  
470438-23-4P 470438-32-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of spiroisoquinoline compds. as SK channel blockers and acetylcholinesterase inhibitors for treatment of constipation)

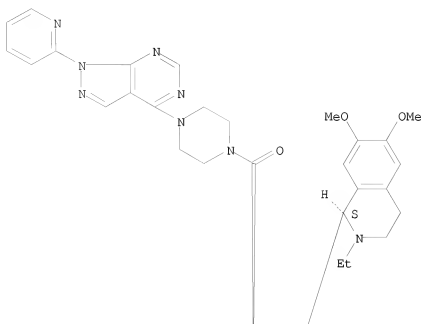
RN 470428-98-9 CAPLUS

CN Carbamic acid, [3-[(1R,2R,4R)-2-[(1S)-2-ethyl-1,2,3,4-tetrahydro-6,7-dimethoxy-1-isoquinolinyl]-3',4'-dihydro-6',7'-dimethoxy-4-[[4-[1-(2-pyridinyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]-1-piperazinyl]carbonyl]spiro[cyclohexane-1,1'(2'H)-isoquinolin]-2'-yl]-3-oxopropyl]methyl-, phenylmethyl ester, rel- (9CI) (CA INDEX NAME)

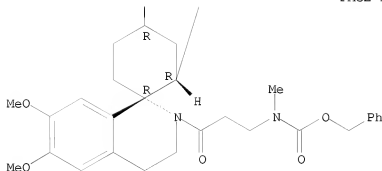


Relative stereochemistry.

PAGE 1-A



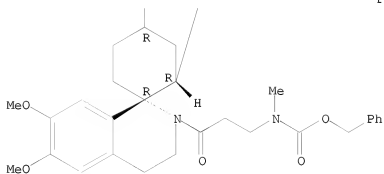
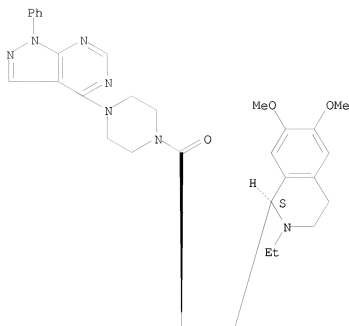
PAGE 2-A



RN 470429-07-3 CAPLUS

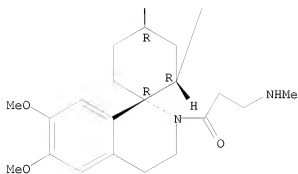
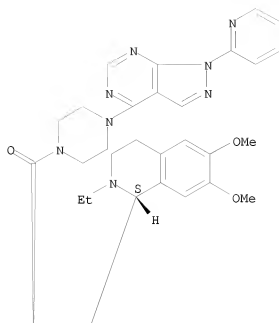
CN Carbamic acid, [3-[(1R,2R,4R)-2-[(1S)-2-ethyl-1,2,3,4-tetrahydro-6,7-dimethoxy-1-isoquinolinyl]-3',4'-dihydro-6',7'-dimethoxy-4-[[4-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-1-piperazinyl]carbonyl]spiro[cyclohexane-1,1'-(2'H)-isoquinolin]-2'-yl]-3-oxopropyl]methyl-, phenylmethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



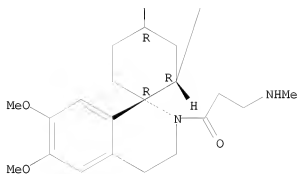
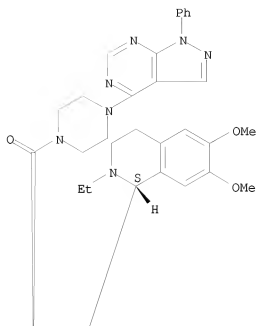
RN 470430-40-1 CAPLUS  
 CN Spiro[cyclohexane-1,1'-(2'H)-isoquinoline], 2-[(1R)-2-ethyl-1,2,3,4-tetrahydro-6,7-dimethoxy-1-isoquinolinyl]-3',4'-dihydro-6',7'-dimethoxy-2'-[3-(methylamino)-1-oxopropyl]-4-[[4-[1-(2-pyridinyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]-1-piperazinyl]carbonyl]-, (1S,2S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 470430-49-0 CAPLUS  
 CN Spiro[cyclohexane-1,1'(2'H)-isoquinolinyl], 2-[(1R)-2-ethyl-1,2,3,4-tetrahydro-6,7-dimethoxy-1-isoquinolinyl]-3',4'-dihydro-6',7'-dimethoxy-2'-[3-(methylamino)-1-oxopropyl]-4-[[4-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-1-piperazinyl]carbonyl]-, (1S,2S,4S)-rel- (9CI) (CA INDEX NAME)

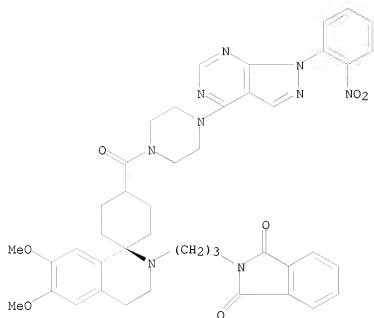
Relative stereochemistry.



RN 470432-18-9 CAPLUS

CN Piperazine, 1-[trans-2'-[3-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)propyl]-3',4'-dihydro-6',7'-dimethoxyspiro[cyclohexane-1,1'(2'H)-isoquinolin]-4-yl]carbonyl]-4-[1-(2-nitrophenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

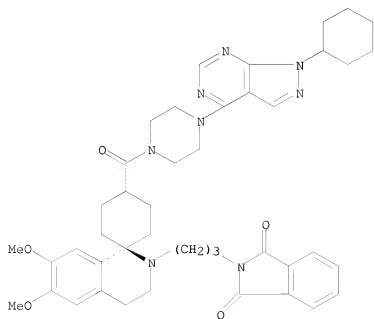
Relative stereochemistry.



RN 470432-22-5 CAPLUS

CN Piperazine, 1-[(1-cyclohexyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-4-[[trans-2'-[3-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)propyl]-3',4'-dihydro-6',7'-dimethoxyspiro[cyclohexane-1,1'-(2'H)-isoquinolin]-4-yl]carbonyl]- (9CI)  
(CA INDEX NAME)

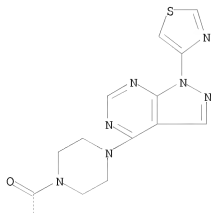
Relative stereochemistry.



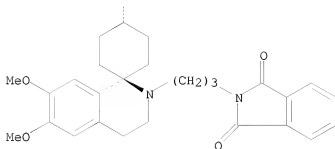
RN 470432-36-1 CAPLUS  
 CN Piperazine, 1-[[trans-2'-[3-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)propyl]-3',4'-dihydro-6',7'-dimethoxyspiro[cyclohexane-1,1'(2'H)-isoquinolin]-4-yl]carbonyl]-4-[1-(4-thiazolyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 2-A

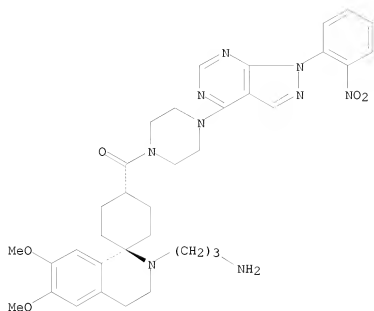


RN 470432-93-0 CAPLUS  
 CN Piperazine, 1-[[trans-2'-[(3-aminopropyl)-3',4'-dihydro-6',7'-dimethoxyspiro[cyclohexane-1,1'(2'H)-isoquinolin]-4-yl]carbonyl]-4-[1-(2-nitrophenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 470432-92-9  
 CMF C35 H43 N9 O5

Relative stereochemistry.



CM 2

CRN 110-17-8  
 CMF C4 H4 O4

Double bond geometry as shown.

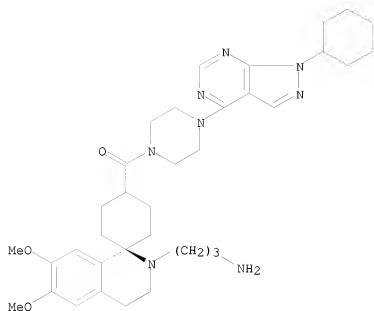


RN 470433-01-3 CAPLUS  
 CN Piperazine, 1-[[trans-2'-(3-aminopropyl)-3',4'-dihydro-6',7'-dimethoxyspiro[cyclohexane-1,1'-(2'H)-isoquinolin]-4-yl]carbonyl]-4-(1-cyclohexyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 470433-00-2  
 CMF C35 H50 N8 O3

Relative stereochemistry.



CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



RN 470438-23-4 CAPLUS

CN Spiro[cyclohexane-1,1'-(2'H)-isoquinoline], 2-[(1R)-2-ethyl-1,2,3,4-tetrahydro-6,7-dimethoxy-1-isoquinolinyl]-3',4'-dihydro-6',7'-dimethoxy-2'-[3-(methylamino)-1-oxopropyl]-4-[[4-[1-(2-pyridinyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]-1-piperazinyl]carbonyl]-, (1S,2S,4S)-rel-, (2E)-2-butenedioate (1:2) (9CI) (CA INDEX NAME)

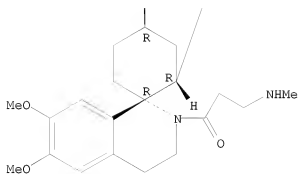
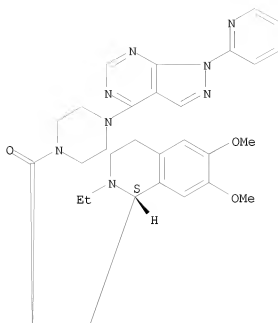
CM 1

CRN 470430-40-1

CMF C48 H60 N10 O6

Relative stereochemistry.



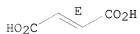


CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



RN 470438-32-5 CAPLUS

CN Spiro[cyclohexane-1,1'(2'H)-isoquinoline], 2-[(1R)-2-ethyl-1,2,3,4-

tetrahydro-6,7-dimethoxy-1-isoquinolinyl]-3',4'-dihydro-6',7'-dimethoxy-2'-  
[3-(methylamino)-1-oxopropyl]-4-[[4-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-  
4-yl)-1-piperazinyl]carbonyl]-, (1S,2S,4S)-rel-, (2E)-2-butenedioate (1:2)  
(9CI) (CA INDEX NAME)

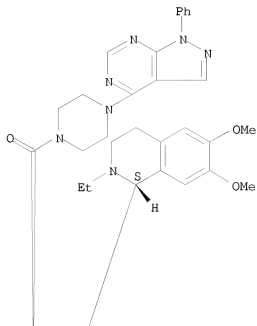
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CRN 470430-49-0

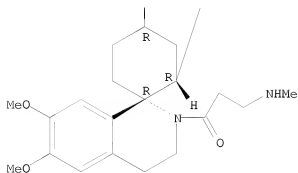
CMF C49 H61 N9 O6

Relative stereochemistry.

PAGE 1-A



PAGE 2-A



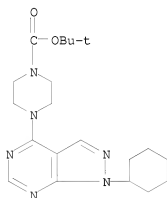
CM 2

CRN 110-17-8  
CMF C4 H4 O4

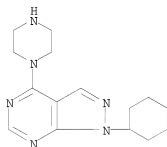
Double bond geometry as shown.



IT 470442-31-0P 470442-42-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(intermediate; preparation of spiroisoquinoline compds. as SK channel  
blockers and acetylcholinesterase inhibitors for treatment of  
constipation)  
RN 470442-31-0 CAPLUS  
CN 1-Piperazinecarboxylic acid, 4-(1-cyclohexyl-1H-pyrazolo[3,4-d]pyrimidin-4-  
yl)-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 470442-42-3 CAPLUS  
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-cyclohexyl-4-(1-piperazinyl)-,  
dihydrochloride (9CI) (CA INDEX NAME)



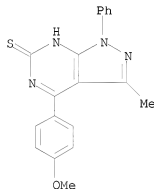
● 2 HCl

GI

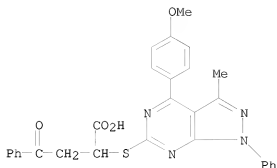
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The invention provides a novel spiroisoquinoline derivative, which has a small-conductance potassium channel (SK) blocking activity and is useful as a medicament, a method for preparing the same, and an intermediate thereof. Specifically, the invention provides spirocyclic compds. I and their pharmaceutically acceptable salts [wherein: the benzo ring of the isoquinoline subunit is optionally substituted; R1 = H or -ZR; R = H, optionally substituted lower alkyl, or optionally substituted lower alkenyl; Z = CH2 or CO; R2 = H or optionally substituted heterocyclic group; X = N or CH; R3 = optionally substituted amino or N-containing aliphatic heterocyclic group; Y = CH2 or CO]. The compds. are useful for prophylaxis or treatment of conditions treatable with SK channel blockers, including constipation, irritable bowel syndrome, gastroesophageal reflux disease, and post-operative ileus. They are also useful for treatment of conditions responsive to compds. with both SK channel-blocking and acetylcholinesterase-inhibiting activities, such as gastrointestinal motility disorders, CNS disorders, memory and learning disorders (including Alzheimer's disease), emotional disorders, myotonic muscular dystrophy, and sleep apnea. Over 900 specific examples of I are given. For instance, di-Et malonate was bis-alkylated with tert-Bu acrylate and partially hydrolyzed, giving 4,4-bis(ethoxycarbonyl) pimelic acid. This was bis-amidated with 2 equiv of homoveratrylamine, and the diamide was bis-cyclized using POC13 to give spirocyclic intermediate II. The latter was converted in 7 steps to acid III, which was condensed with 2-amino-4-(piperazin-1-yl)pyridine to give title compound IV. Selected compds. I inhibited 125I-apamine binding to guinea pig colon membrane cells with IC50 values of 0.004 to 0.06  $\mu$ M. Other compds. I inhibited acetylcholinesterase in vitro with IC50 values of 0.00008 to 0.06  $\mu$ M. The oral ED of selected I for promoting evacuation in guinea pigs was 0.1 to 1 mg/kg.

L14 ANSWER 22 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2002:619490 CAPLUS  
 DOCUMENT NUMBER: 138:73223  
 TITLE: Synthesis and reactions of new substituted pyrimidine  
 thione derivatives as antimicrobial agents  
 AUTHOR(S): El-Ghaffar, Nahed F. A. B. D.; Kassab, Rafika R. S.;  
 Soliman, Fekria M. A.  
 CORPORATE SOURCE: Department of Chemistry, Faculty of Science (Girls),  
 Al-Azhar University, Nasr City, Egypt  
 SOURCE: Revue Roumaine de Chimie (2002), Volume Date 2001,  
 46(5), 535-542  
 CODEN: RRCHAX; ISSN: 0035-3930  
 PUBLISHER: Editura Academiei Romane  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 138:73223  
 IT 106924-33-8  
 RL: PAC (Pharmacological activity); RCT (Reactant); BIOL (Biological  
 study); RACT (Reactant or reagent)  
 (synthesis and reactions of new substituted pyrimidine thione derivs.  
 as antimicrobial agents)  
 RN 106924-33-8 CAPLUS  
 CN 6H-Pyrazolo[3,4-d]pyrimidine-6-thione, 1,5-dihydro-4-(4-methoxyphenyl)-3-  
 methyl-1-phenyl- (9CI) (CA INDEX NAME)

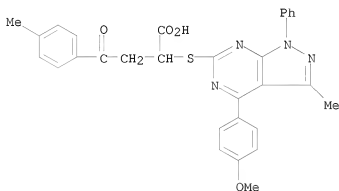


IT 470485-35-9P 470485-36-0P 470485-37-1P  
 470485-39-3P 470485-50-8P 470485-51-9P  
 470485-52-0P 470485-53-1P 470485-54-2P  
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic  
 preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant  
 or reagent)  
 (synthesis and reactions of new substituted pyrimidine thione derivs.  
 as antimicrobial agents)  
 RN 470485-35-9 CAPLUS  
 CN Benzenebutanoic acid,  $\alpha$ -[[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-  
 pyrazolo[3,4-d]pyrimidin-6-yl]thio]- $\gamma$ -oxo- (CA INDEX NAME)



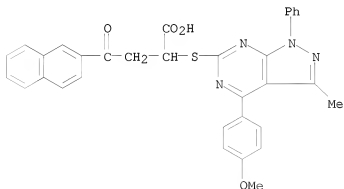
RN 470485-36-0 CAPLUS

CN Benzenebutanoic acid,  $\alpha$ -[[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]thio]-4-methyl- $\gamma$ -oxo- (CA INDEX NAME)



RN 470485-37-1 CAPLUS

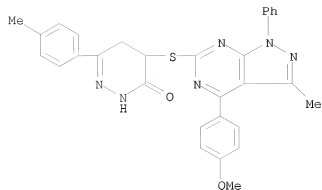
CN 2-Naphthalenebutanoic acid,  $\alpha$ -[[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]thio]- $\gamma$ -oxo- (CA INDEX NAME)



RN 470485-39-3 CAPLUS

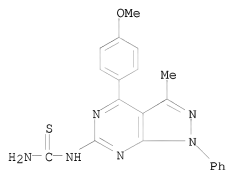
CN 3(2H)-Pyridazinone, 4,5-dihydro-4-[[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]thio]-6-(4-methylphenyl)- (CA INDEX NAME)

NAME)



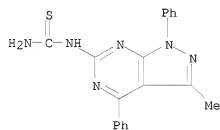
RN 470485-50-8 CAPLUS

CN Thiourea, [4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]- (9CI) (CA INDEX NAME)



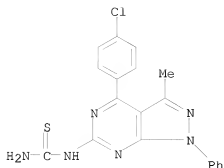
RN 470485-51-9 CAPLUS

CN Thiourea, (3-methyl-1,4-diphenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl)- (9CI) (CA INDEX NAME)



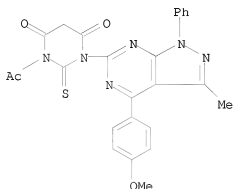
RN 470485-52-0 CAPLUS

CN Thiourea, [4-(4-chlorophenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]- (9CI) (CA INDEX NAME)



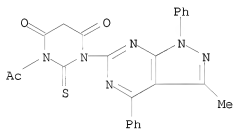
RN 470485-53-1 CAPLUS

CN 4,6 (1H,5H)-Pyrimidinedione, 1-acetyldihydro-3-(4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl)-2-thioxo- (CA INDEX NAME)



RN 470485-54-2 CAPLUS

CN 4,6 (1H,5H)-Pyrimidinedione, 1-acetyldihydro-3-(3-methyl-1,4-diphenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl)-2-thioxo- (CA INDEX NAME)



IT 470485-40-6P 470485-41-7P 470485-42-8P

470485-44-0P 470485-45-1P 470485-46-2P

470485-49-5P 470485-55-3P 470485-56-4P

470485-57-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

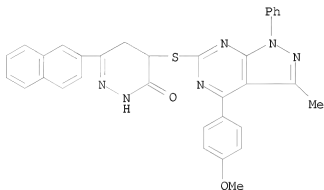
(synthesis and reactions of new substituted pyrimidine thione derivs.



as antimicrobial agents)

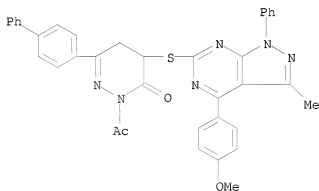
RN 470485-40-6 CAPLUS

CN 3(2H)-Pyridazinone, 4,5-dihydro-4-[[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]thio]-6-(2-naphthalenyl)- (CA INDEX NAME)



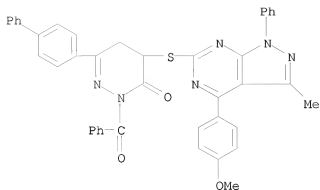
RN 470485-41-7 CAPLUS

CN 3(2H)-Pyridazinone, 2-acetyl-6-[1,1'-biphenyl]-4-yl-4,5-dihydro-4-[[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]thio]- (CA INDEX NAME)



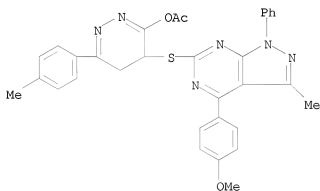
RN 470485-42-8 CAPLUS

CN 3(2H)-Pyridazinone, 2-benzoyl-6-[1,1'-biphenyl]-4-yl-4,5-dihydro-4-[[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]thio]- (CA INDEX NAME)



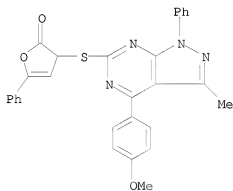
RN 470485-44-0 CAPLUS

CN 3-Pyridazinol, 4,5-dihydro-4-[[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]thio]-6-(4-methylphenyl)-, acetate (ester) (9CI) (CA INDEX NAME)



RN 470485-45-1 CAPLUS

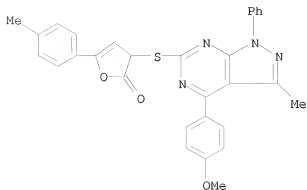
CN 2(3H)-Furanone, 3-[[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]thio]-5-phenyl- (CA INDEX NAME)



RN 470485-46-2 CAPLUS

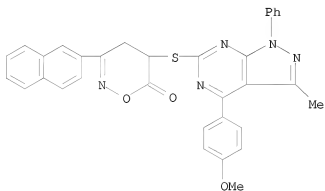
CN 2(3H)-Furanone, 3-[[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-

d]pyrimidin-6-yl]thio]-5-(4-methylphenyl)- (CA INDEX NAME)



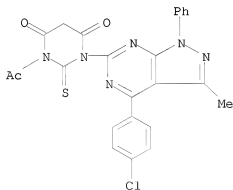
RN 470485-49-5 CAPLUS

CN 6H-1,2-Oxazin-6-one, 4,5-dihydro-5-[[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]thio]-3-(2-naphthalenyl)- (CA INDEX NAME)

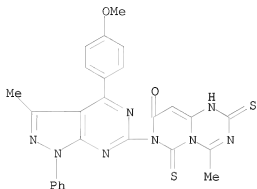


RN 470485-55-3 CAPLUS

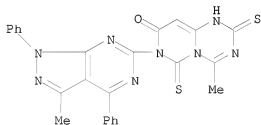
CN 4,6(1H,5H)-Pyrimidinedione, 1-acetyl-3-[4-(4-chlorophenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]dihydro-2-thioxo- (CA INDEX NAME)



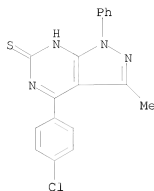
RN 470485-56-4 CAPLUS  
 CN 8H-Pyrimido[1,6-a]-1,3,5-triazin-8-one, 1,2,6,7-tetrahydro-7-[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]-4-methyl-2,6-dithioxo- (CA INDEX NAME)



RN 470485-57-5 CAPLUS  
 CN 8H-Pyrimido[1,6-a]-1,3,5-triazin-8-one, 1,2,6,7-tetrahydro-4-methyl-7-(3-methyl-1,4-diphenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl)-2,6-dithioxo- (CA INDEX NAME)

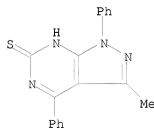


IT 106924-32-7 106936-09-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (synthesis and reactions of new substituted pyrimidine thione derivs.  
 as antimicrobial agents)  
 RN 106924-32-7 CAPLUS  
 CN 6H-Pyrazolo[3,4-d]pyrimidine-6-thione, 4-(4-chlorophenyl)-1,5-dihydro-3-methyl-1-phenyl- (9CI) (CA INDEX NAME)



RN 106936-09-8 CAPLUS

CN 6H-Pyrazolo[3,4-d]pyrimidine-6-thione, 1,5-dihydro-3-methyl-1,4-diphenyl-(9CI) (CA INDEX NAME)

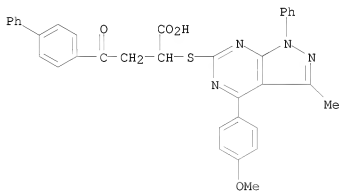


IT 470485-38-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(synthesis and reactions of new substituted pyrimidine thione derivs.  
as antimicrobial agents)

RN 470485-38-2 CAPLUS

CN [1,1'-Biphenyl]-4-butanoic acid,  $\alpha$ -[[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]thio]- $\gamma$ -oxo- (CA INDEX NAME)

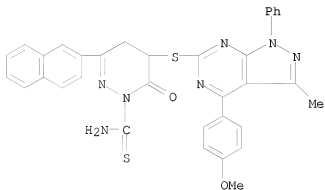


IT 470485-43-9P 470485-47-3P 470485-48-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (synthesis and reactions of new substituted pyrimidine thione derivs.  
 as antimicrobial agents)

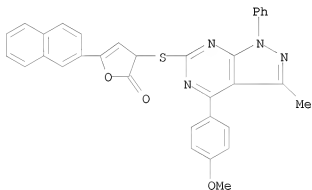
RN 470485-43-9 CAPLUS

CN 1(4H)-Pyridazinecarbothioamide, 5,6-dihydro-5-[[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]thio]-3-(2-naphthalenyl)-6-oxo- (CA INDEX NAME)



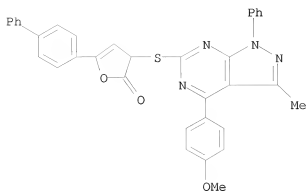
RN 470485-47-3 CAPLUS

CN 2(3H)-Furanone, 3-[[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]thio]-5-(2-naphthalenyl)- (CA INDEX NAME)

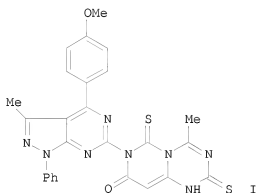


RN 470485-48-4 CAPLUS

CN 2(3H)-Furanone, 5-[1,1'-biphenyl]-4-yl-3-[[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]thio]- (CA INDEX NAME)



GI



AB Pyrimidinethiones containing also other heterocyclic moieties are known to exhibit varied biol. and pharmacol. properties. In view of these observations, the present work describes the synthesis of some new substituted pyrimidine thiones, e.g. I, starting from  $\alpha$ ,  $\beta$ -unsatd. carbonyl compds. and their antimicrobial activities. An attempt is made to study the structural activity relationships.

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 23 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:325908 CAPLUS

DOCUMENT NUMBER: 137:257233

TITLE: Pyrazolopyrimidines: synthesis, effect on histamine release from rat peritoneal mast cells and cytotoxic activity

AUTHOR(S): Quintela, Jose M.; Peinador, Carlos; Moreira, Maria J.; Alfonso, Amparo; Botana, Luis M.; Rigüera, Ricardo  
CORPORATE SOURCE: Departamento de Química Fundamental e Industrial, Facultad de Ciencias, Universidad de La Coruña, La Coruña, E-15071, Spain

SOURCE: European Journal of Medicinal Chemistry (2001), 36(4), 321-332

CODEN: EJMCAS; ISSN: 0223-5234

PUBLISHER: Editions Scientifiques et Medicales Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

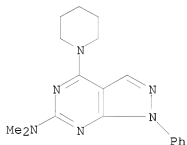
OTHER SOURCE(S): CASREACT 137:257233

IT 461670-40-6P 461670-42-8P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(pyrazolopyrimidines: synthesis and effect on histamine release from rat peritoneal mast cells and cytotoxic activity)

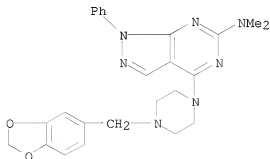
RN 461670-40-6 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidin-6-amine, N,N-dimethyl-1-phenyl-4-(1-piperidinyl)- (CA INDEX NAME)



RN 461670-42-8 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidin-6-amine, 4-[4-(1,3-benzodioxol-5-ylmethyl)-1-piperazinyl]-N,N-dimethyl-1-phenyl- (CA INDEX NAME)





IT 461670-61-1P 461670-62-2P

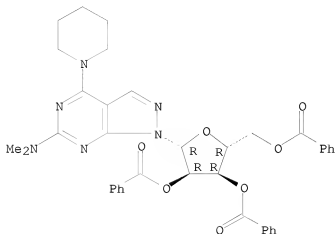
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(pyrazolopyrimidines: synthesis and effect on histamine release from rat peritoneal mast cells and cytotoxic activity)

RN 461670-61-1 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidin-6-amine, N,N-dimethyl-4-(1-piperidinyl)-1-(2,3,5-tri-O-benzoyl-β-D-ribofuranosyl)- (CA INDEX NAME)

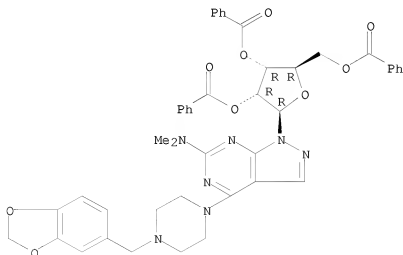
Absolute stereochemistry.



RN 461670-62-2 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidin-6-amine, 4-[4-(1,3-benzodioxol-5-ylmethyl)-1-piperazinyl]-N,N-dimethyl-1-(2,3,5-tri-O-benzoyl-β-D-ribofuranosyl)- (CA INDEX NAME)

Absolute stereochemistry.



AB A series of 1H-pyrazolo[3,4-d]pyrimidines substituted at positions 1 (R1 = Ph, H, tert-Bu and ribosetribenzoate), 4 (R2 = chlorine, nitrogen and

oxygen nucleophiles), and 6 (dimethylamino) have been synthesized and their effect on the release of histamine from rat peritoneal mast cells measured. After chemical stimulation, (polymer 48/80), several compds., produce inhibition two to three times higher (40-60%) than DSCG but this action is lower after preincubation. Some of the compds. (where R1 = Ph, R2 = NHCH2Ph; 50-70% inhibition) or (where R1 = H, R2 = OMe; 50-55% inhibition) are the most active ones in both expts. With ovalbumin as stimulus, several pyrazolopyrimidines show inhibition similar to DSCG. Some of the compds. (where R1 = t-Bu, R2 = OMe) or ( where R1 = t-Bu, R2 = piperidino) are inducers of the release of histamine (60 and 150% increase). Some compds. showed cytotoxic activity (IC50 = 1 µg/mL) to HT-29 human colon cancer cells.

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 24 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:75029 CAPLUS

DOCUMENT NUMBER: 137:310880

TITLE: Synthesis and reactions of new substituted pyrimidine thione derivatives as antimicrobial agents

AUTHOR(S): Abd El-Ghaffar, Nahed F.; Kassab, Rafika R. S.; Soliman, Fekria M. A.

CORPORATE SOURCE: Department of Chemistry, Faculty of Science (Girls) Al-Azhar University, Nasr City, Egypt

SOURCE: Al-Azhar Bulletin of Science (2000), 11(1), 161-170

CODEN: ABSCE7; ISSN: 1110-2535

PUBLISHER: Al-Azhar University, Faculty of Science

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:310880

IT 470485-35-9P 470485-36-0P 470485-37-1P

470485-39-3P 470485-50-8P 470485-51-9P

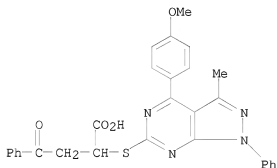
470485-52-0P 470485-53-1P 470485-54-2P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(preparation, antimicrobial activity, and structure-activity relationship of substituted pyrimidinethiones)

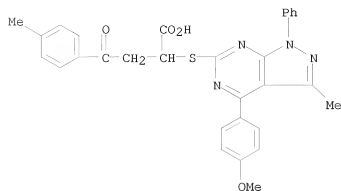
RN 470485-35-9 CAPLUS

CN Benzenebutanoic acid,  $\alpha$ -[[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]thio]- $\gamma$ -oxo- (CA INDEX NAME)



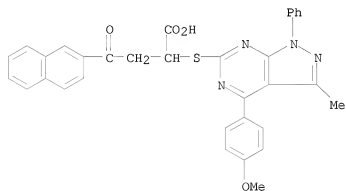
RN 470485-36-0 CAPLUS

CN Benzenebutanoic acid,  $\alpha$ -[[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]thio]-4-methyl- $\gamma$ -oxo- (CA INDEX NAME)



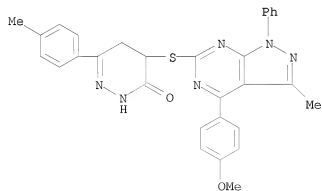
RN 470485-37-1 CAPLUS

CN 2-Naphthalenebutanoic acid,  $\alpha$ -[[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]thio]- $\gamma$ -oxo- (CA INDEX NAME)



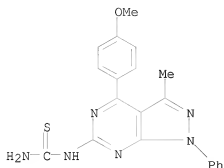
RN 470485-39-3 CAPLUS

CN 3(2H)-Pyridazinone, 4,5-dihydro-4-[[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]thio]-6-(4-methylphenyl)- (CA INDEX NAME)



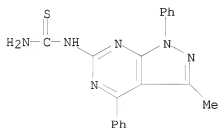
RN 470485-50-8 CAPLUS

CN Thiourea, [4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]- (9CI) (CA INDEX NAME)



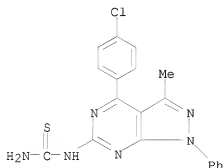
RN 470485-51-9 CAPLUS

CN Thiourea, (3-methyl-1,4-diphenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl)- (9CI) (CA INDEX NAME)



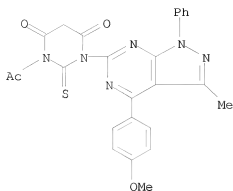
RN 470485-52-0 CAPLUS

CN Thiourea, [4-(4-chlorophenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]- (9CI) (CA INDEX NAME)



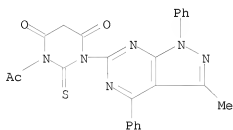
RN 470485-53-1 CAPLUS

CN 4,6(1H,5H)-Pyrimidinedione, 1-acetyldihydro-3-[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]-2-thioxo- (CA INDEX NAME)



RN 470485-54-2 CAPLUS

CN 4,6(1H,5H)-Pyrimidinedione, 1-acetyldihydro-3-(3-methyl-1,4-diphenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl)-2-thioxo- (CA INDEX NAME)



IT 470485-40-6P 470485-41-7P 470485-42-8P

470485-44-0P 470485-45-1P 470485-46-2P

470485-49-5P 470485-55-3P 470485-56-4P

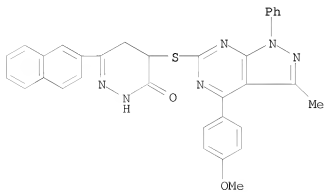
470485-57-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation, antimicrobial activity, and structure-activity relationship of substituted pyrimidinethiones)

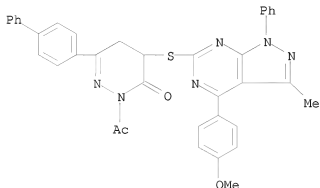
RN 470485-40-6 CAPLUS

CN 3(2H)-Pyridazinone, 4,5-dihydro-4-[[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]thio]-6-(2-naphthalenyl)- (CA INDEX NAME)



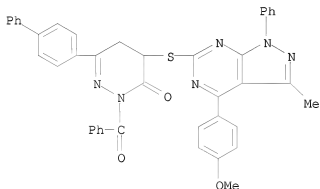
RN 470485-41-7 CAPLUS

CN 3(2H)-Pyridazinone, 2-acetyl-6-[1,1'-biphenyl]-4-yl-4,5-dihydro-4-[[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]thio]-  
(CA INDEX NAME)



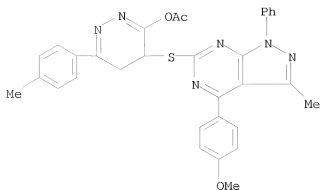
RN 470485-42-8 CAPLUS

CN 3(2H)-Pyridazinone, 2-benzoyl-6-[1,1'-biphenyl]-4-yl-4,5-dihydro-4-[[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]thio]-  
(CA INDEX NAME)



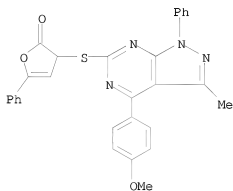
RN 470485-44-0 CAPLUS

CN 3-Pyridazinol, 4,5-dihydro-4-[[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]thio]-6-(4-methylphenyl)-, acetate (ester)  
(9CI) (CA INDEX NAME)



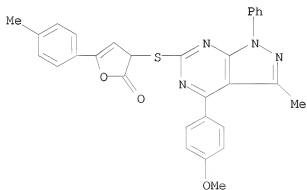
RN 470485-45-1 CAPLUS

CN 2-(3H)-Furanone, 3-[[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]thio]-5-phenyl- (CA INDEX NAME)



RN 470485-46-2 CAPLUS

CN 2-(3H)-Furanone, 3-[[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]thio]-5-(4-methylphenyl)- (CA INDEX NAME)

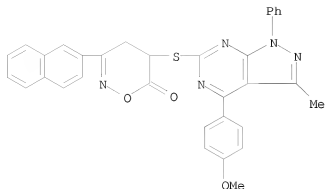


RN 470485-49-5 CAPLUS

CN 6H-1,2-Oxazin-6-one, 4,5-dihydro-5-[[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]thio]-3-(2-naphthalenyl)- (CA INDEX NAME)

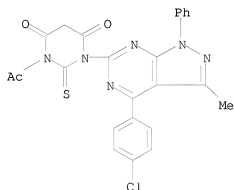


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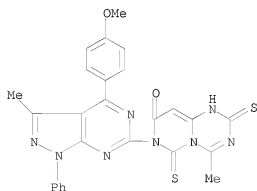
RN 470485-55-3 CAPLUS

CN 4,6(1H,5H)-Pyrimidinedione, 1-acetyl-3-[4-(4-chlorophenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]dihydro-2-thioxo- (CA INDEX NAME)

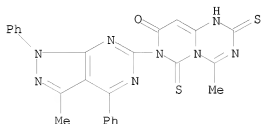


RN 470485-56-4 CAPLUS

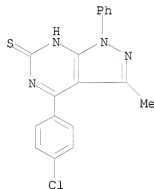
CN 8H-Pyrimido[1,6-a]-1,3,5-triazin-8-one, 1,2,6,7-tetrahydro-7-[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]-4-methyl-2,6-dithioxo- (CA INDEX NAME)



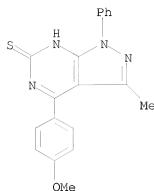
RN 470485-57-5 CAPLUS  
 CN 8H-Pyrimido[1,6-a]-1,3,5-triazin-8-one, 1,2,6,7-tetrahydro-4-methyl-7-(3-methyl-1,4-diphenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl)-2,6-dithioxo- (CA INDEX NAME)



IT 106924-32-7 106924-33-8 106936-09-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation, antimicrobial activity, and structure-activity relationship of substituted pyrimidinethiones)  
 RN 106924-32-7 CAPLUS  
 CN 6H-Pyrazolo[3,4-d]pyrimidine-6-thione, 4-(4-chlorophenyl)-1,5-dihydro-3-methyl-1-phenyl- (9CI) (CA INDEX NAME)

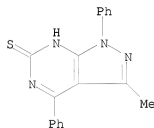


RN 106924-33-8 CAPLUS  
 CN 6H-Pyrazolo[3,4-d]pyrimidine-6-thione, 1,5-dihydro-4-(4-methoxyphenyl)-3-methyl-1-phenyl- (9CI) (CA INDEX NAME)



RN 106936-09-8 CAPLUS

CN 6H-Pyrazolo[3,4-d]pyrimidine-6-thione, 1,5-dihydro-3-methyl-1,4-diphenyl-  
(9CI) (CA INDEX NAME)

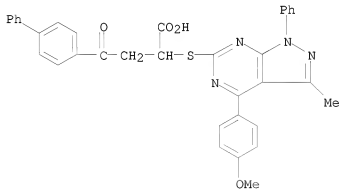


IT 470485-38-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation, antimicrobial activity, and structure-activity relationship of  
substituted pyrimidinethiones)

RN 470485-38-2 CAPLUS

CN [1,1'-Biphenyl]-4-butanoic acid,  $\alpha$ -[[4-(4-methoxyphenyl)-3-methyl-1-  
phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]thio]- $\gamma$ -oxo- (CA INDEX  
NAME)

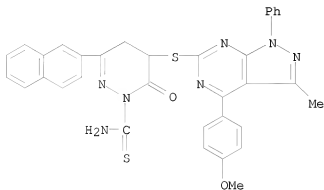


IT 470485-43-9P 470485-47-3P 470485-48-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation, antimicrobial activity, and structure-activity relationship of  
substituted pyrimidinethiones)

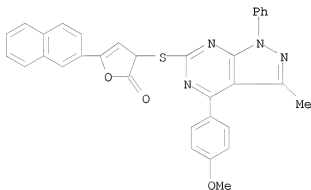
RN 470485-43-9 CAPLUS

CN 1(4H)-Pyridazinecarbothioamide, 5,6-dihydro-5-[[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]thio]-3-(2-naphthalenyl)-6-oxo- (CA INDEX NAME)



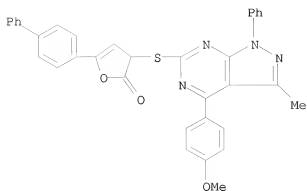
RN 470485-47-3 CAPLUS

CN 2(3H)-Furanone, 3-[[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]thio]-5-(2-naphthalenyl)- (CA INDEX NAME)

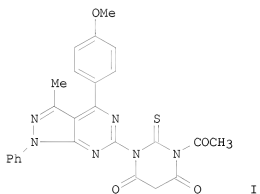


RN 470485-48-4 CAPLUS

CN 2(3H)-Furanone, 5-[1,1'-biphenyl]-4-yl-3-[[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]thio]- (CA INDEX NAME)



GI

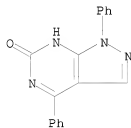


I

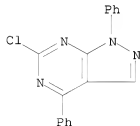
AB Pyrimidinethiones, e.g., I, containing other heterocyclic moieties are known to exhibit varied biol. and pharmacol. properties. In view of these observations, the present work describes the synthesis of some new substituted pyrimidinethiones starting from  $\alpha,\beta$ -unsatd. carbonyl compds. and evaluation of their antimicrobial activities. An attempt is made to study the structural activity relationships.

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

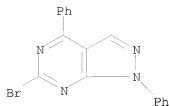
L14 ANSWER 25 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2001:418164 CAPLUS  
 DOCUMENT NUMBER: 135:166522  
 TITLE: Application of phosphonium salts to the reactions of various kinds of amides  
 AUTHOR(S): Sugimoto, Osamu; Mori, Miho; Moriya, Keisuke; Tanji, Ken-Ichi  
 CORPORATE SOURCE: Laboratory of Organic Chemistry, School of Food and Nutritional Sciences, University of Shizuoka, Shizuoka, 422-8526, Japan  
 SOURCE: Helvetica Chimica Acta (2001), 84(5), 1112-1118  
 CODEN: HCACAV; ISSN: 0018-019X  
 PUBLISHER: Verlag Helvetica Chimica Acta  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 135:166522  
 IT 35026-01-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (halogenation of electron-deficient heteroarom. alcs. by phosphonium salts)  
 RN 35026-01-8 CAPLUS  
 CN 6H-Pyrazolo[3,4-d]pyrimidin-6-one, 1,5-dihydro-1,4-diphenyl- (9CI) (CA INDEX NAME)



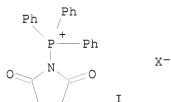
IT 35016-14-9P 354574-57-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (halogenation of electron-deficient heteroarom. alcs. by phosphonium salts)  
 RN 35016-14-9 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-chloro-1,4-diphenyl- (CA INDEX NAME)



RN 354574-57-5 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-bromo-1,4-diphenyl- (CA INDEX NAME)



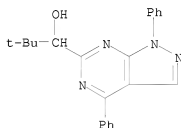
GI



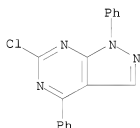
AB The phosphonium salts I ( $X = \text{Cl}, \text{Br}$ ), prepared from triphenylphosphine and N-halosuccinimide, proved to be applicable to the conversion of amide compds. Especially, halogenation of electron-deficient heteroarom. alcs. with these reagents seems to be a convenient method compared to the halogenation with phosphorus oxyhalides.

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 26 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2001:178044 CAPLUS  
 DOCUMENT NUMBER: 134:353268  
 TITLE: The tellurium-lithium exchange reaction: selective functionalization of electron-deficient heteroaromatics  
 AUTHOR(S): Sugimoto, O.; Sudo, M.; Tanji, K.-i.  
 CORPORATE SOURCE: School of Food and Nutritional Sciences, Laboratory of Organic Chemistry, University of Shizuoka, Shizuoka, 422-8526, Japan  
 SOURCE: Tetrahedron (2001), 57(11), 2133-2138  
 CODEN: TETRAB; ISSN: 0040-4020  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 134:353268  
 IT 339305-67-8P  
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)  
 RN 339305-67-8 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine-6-methanol,  $\alpha$ -(1,1-dimethylethyl)-1,4-diphenyl- (CA INDEX NAME)

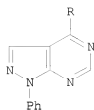


IT 35016-14-9  
 RL: RCT (Reactant); RACT (Reactant or reagent) (reaction with lithium butanetellurolate)  
 RN 35016-14-9 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-chloro-1,4-diphenyl- (CA INDEX NAME)



GI





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AB Electron-deficient heteroarom. tellurides, which was obtained from the corresponding haloheteroaroms., reacted selectively with n-butyllithium to give the lithio derivs. Thus, reaction of 4-chloro-1-phenyl-1H-pyrazolo[3,4-d]pyrimidine I (R = Cl) with lithium butanetellurolate gave 90% I (R = BuTe) which on lithiation with BuLi followed by treatment with pivaldehyde and hydrolysis gave 52% I (R = CH(OHBu-t)).

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 27 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:646012 CAPLUS

DOCUMENT NUMBER: 133:222742

TITLE: Preparation of carbamoyltetrahydropyridine derivs. for treatment of CRF-related diseases

INVENTOR(S): Nakazato, Atsuro; Okubo, Taketoshi; Kumagai, Toshihito; Tomisawa, Kazuyuki

PATENT ASSIGNEE(S): Taisho Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 51 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000053604	A1	20000914	WO 2000-JP1468	20000310
W: AU, CA, CN, KR, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2366642	A1	20000914	CA 2000-2366642	20000310
JP 2001151777	A	20010605	JP 2000-66205	20000310
EP 1176146	A1	20020130	EP 2000-907999	20000310
EP 1176146	B1	20050608		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
AU 756702	B2	20030123	AU 2000-29414	20000310
EP 1449843	A1	20040825	EP 2004-5593	20000310
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
AT 297393	T	20050615	AT 2000-907999	20000310
ES 2239592	T3	20051001	ES 2000-907999	20000310
US 6600038	B1	20030729	US 2001-914534	20010830
HK 1046683	A1	20050520	HK 2002-108223	20021113
US 20030191122	A1	20031009	US 2003-347288	20030121
US 6894168	B2	20050517		

PRIORITY APPLN. INFO.:

JP 1999-65004	A	19990311
JP 1999-185628	A	19990630
JP 1999-258353	A	19990913
EP 2000-907999	A3	20000310
WO 2000-JP1468	W	20000310
US 2001-914534	A3	20010830

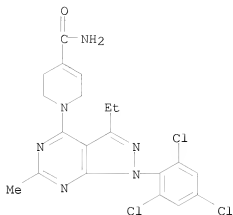
OTHER SOURCE(S): MARPAT 133:222742

IT 291538-41-5P 291538-42-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of carbamoyltetrahydropyridine derivs. for treatment of CRF-related diseases)

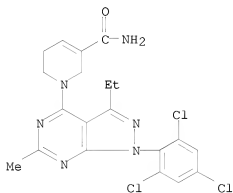
RN 291538-41-5 CAPLUS

CN 4-Pyridinecarboxamide, 1-[3-ethyl-6-methyl-1-(2,4,6-trichlorophenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]-1,2,3,6-tetrahydro- (CA INDEX NAME)

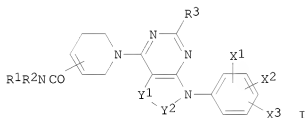


RN 291538-42-6 CAPLUS

CN 3-Pyridinecarboxamide, 1-[3-ethyl-6-methyl-1-(2,4,6-trichlorophenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]-1,2,5,6-tetrahydro- (CA INDEX NAME)



GI



AB Title compds. I (R1, R2 = H, alkyl; R1R2N = morpholino, pyrrolidino; R3 = H, alkyl; Y1-Y2 = R4C=CR5, R6C=N, N=N, R7N-CO, N=CR8; X1, X2, X3 = H, halo, alkyl, alkoxy, alkylthio, etc; R4, R5, R6 = H, alkyl, etc.; R7 = H, alkyl, alkoxy, carbonylmethyl, etc.; R8 = H, carbamoyl) and their medicinally acceptable salts, are prepared Thus, 4-(4-carbamoyl-1,2,3,6-

tetrahydropyridin-1-yl)-2,5-dimethyl-7-(4-isopropyl-2-methylthiophenyl)-7H-pyrrolo[2,3-d]pyrimidine was prepared in several steps from Et 1-methyl-1,2,3,6-tetrahydropyridine-4-carboxylate and showed IC50 of  $\leq 100$  nM CRF receptor binding activity when tested with rat.

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 28 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2000:568540 CAPLUS  
 DOCUMENT NUMBER: 133:164062  
 TITLE: Preparation of pyrazoles and pyrazolopyrimidines  
 having CRF antagonistic activity  
 INVENTOR(S): Faraci, William Stephen; Welch, Willard Mckowan, Jr.  
 PATENT ASSIGNEE(S): Pfizer Inc., USA  
 SOURCE: U.S., 22 pp.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 3  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6103900	A	20000815	US 1997-961413	19971030
US 20020049227	A1	20020425	US 1999-377569	19990819
US 6448265	B2	20020910		

PRIORITY APPLN. INFO.:  
 US 1992-992225 B3 19921217  
 WO 1993-US10359 W 19931103  
 US 1995-448529 A3 19950614  
 US 1997-961413 A3 19971030

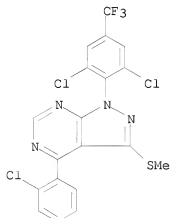
OTHER SOURCE(S): MARPAT 133:164062

IT 157434-80-5P 157434-81-6P 157434-82-7P  
 157434-83-8P 157434-84-9P 157434-85-0P  
 157434-86-1P 157434-87-2P 157434-88-3P  
 157434-89-4P 157434-90-7P 157434-91-8P  
 157434-92-9P 157434-93-0P 157434-94-1P  
 157434-95-2P 157434-96-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of pyrazoles and pyrazolopyrimidines having CRF antagonistic activity)

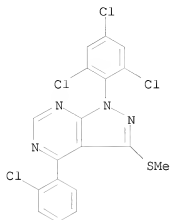
RN 157434-80-5 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(2-chlorophenyl)-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-3-(methylthio)- (CA INDEX NAME)



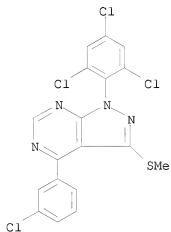
RN 157434-81-6 CAPLUS

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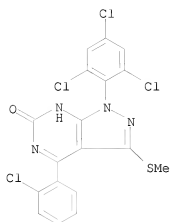
RN 157434-82-7 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(3-chlorophenyl)-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



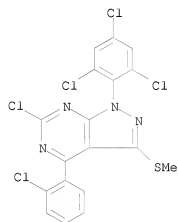
RN 157434-83-8 CAPLUS

CN 6H-Pyrazolo[3,4-d]pyrimidin-6-one, 4-(2-chlorophenyl)-1,5-dihydro-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (9CI) (CA INDEX NAME)



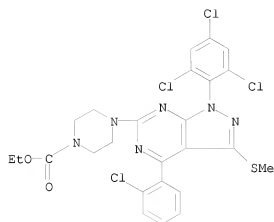
RN 157434-84-9 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-chloro-4-(2-chlorophenyl)-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



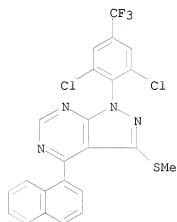
RN 157434-85-0 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[4-(2-chlorophenyl)-3-(methylthio)-1-(2,4,6-trichlorophenyl)-1H-pyrazolo[3,4-d]pyrimidin-6-yl]-, ethyl ester (CA INDEX NAME)



RN 157434-86-1 CAPLUS

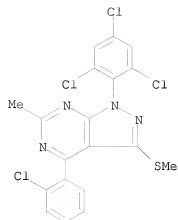
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-3-(methylthio)-4-(1-naphthalenyl)- (CA INDEX NAME)



RN 157434-87-2 CAPLUS

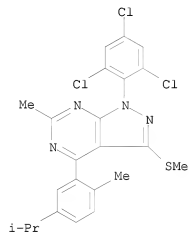
CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(2-chlorophenyl)-6-methyl-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)





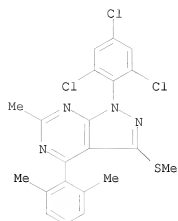
RN 157434-88-3 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-methyl-4-[2-methyl-5-(1-methylethyl)phenyl]-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



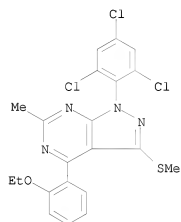
RN 157434-89-4 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(2,6-dimethylphenyl)-6-methyl-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



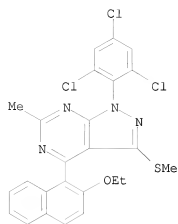
RN 157434-90-7 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(2-ethoxyphenyl)-6-methyl-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



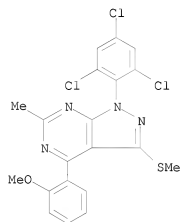
RN 157434-91-8 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(2-ethoxy-1-naphthalenyl)-6-methyl-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



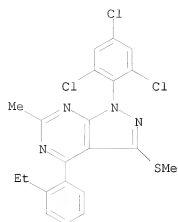
RN 157434-92-9 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(2-methoxyphenyl)-6-methyl-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



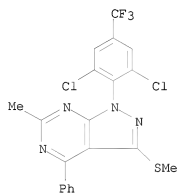
RN 157434-93-0 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(2-ethylphenyl)-6-methyl-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



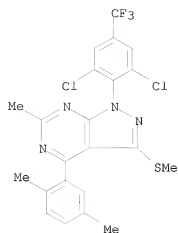
RN 157434-94-1 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-6-methyl-3-(methylthio)-4-phenyl- (CA INDEX NAME)



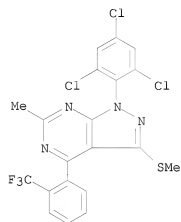
RN 157434-95-2 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(2,5-dimethylphenyl)-6-methyl-3-(methylthio)- (CA INDEX NAME)

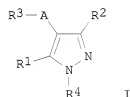


RN 157434-96-3 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-methyl-3-(methylthio)-1-(2,4,6-trichlorophenyl)-4-[2-(trifluoromethyl)phenyl]- (CA INDEX NAME)



GI



AB The title compds. [I; A and R1 together with the carbons to which they are attached form (un)substituted pyrimidinyl; A = CO; R1 = NH2; R2 = H,

alkyl, OH, etc.; R3 = (un)substituted Ph, naphthyl, 3-8 membered cycloalkyl, etc.; R4 = 2,4,6-Cl3C6H2; 2,4,6-Me3C6H2, 2,6-Cl2-4-F3CC6H2, 4-Br-2,6-Me2C6H2] which have corticotropin releasing factor (CRF) antagonist activity, and therefore are effective in the treatment of a wide range of diseases including stress-related illnesses, were prepared E.g., a multi-step synthesis of I [A = CO; R1 = NH2; R2 = SMe; R3 = 2,5-Me2C6H3; R4 = 2,6-Cl2-4-F3CC6H2] was given. The binding activity of compds. I to a CRF receptor generally ranges from 0.2 nM - 10  $\mu$ M.

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 29 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:808685 CAPLUS  
DOCUMENT NUMBER: 132:35715  
TITLE: Preparation of pyrazoles and pyrazolopyrimidines  
having CRF antagonistic activity  
INVENTOR(S): Faraci, William Stephen; Welch, Willard McKowan, Jr.  
PATENT ASSIGNEE(S): Pfizer Inc., USA  
SOURCE: U.S., 19 pp.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 3  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 6005109	A	19991221	US 1997-961414	19971030
US 20020016333	A1	20020207	US 1999-377350	19990819
US 6441018	B2	20020827		

PRIORITY APPLN. INFO.:  
US 1992-992225 B2 19921217  
WO 1993-US10359 W 19931103  
US 1995-448529 A3 19950614  
US 1997-961414 A3 19971030

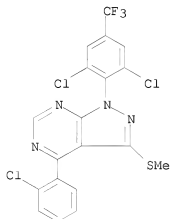
OTHER SOURCE(S): MARPAT 132:35715

IT 157434-80-5P 157434-81-6P 157434-82-7P  
157434-83-8P 157434-84-9P 157434-85-0P  
157434-86-1P 157434-87-2P 157434-88-3P  
157434-89-4P 157434-90-7P 157434-91-8P  
157434-92-9P 157434-93-0P 157434-94-1P  
157434-95-2P 157434-96-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of pyrazoles and pyrazolopyrimidines having CRF antagonistic activity)

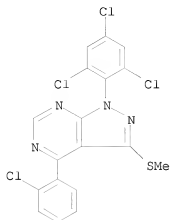
RN 157434-80-5 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(2-chlorophenyl)-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-3-(methylthio)- (CA INDEX NAME)



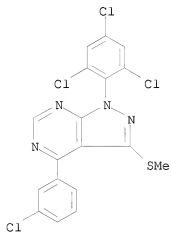
RN 157434-81-6 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(2-chlorophenyl)-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



RN 157434-82-7 CAPLUS

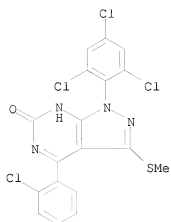
CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(3-chlorophenyl)-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



RN 157434-83-8 CAPLUS

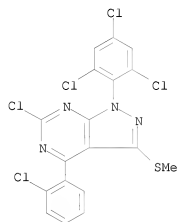
CN 6H-Pyrazolo[3,4-d]pyrimidin-6-one, 4-(2-chlorophenyl)-1,5-dihydro-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (9CI) (CA INDEX NAME)





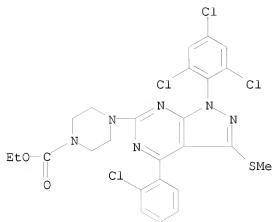
RN 157434-84-9 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-chloro-4-(2-chlorophenyl)-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



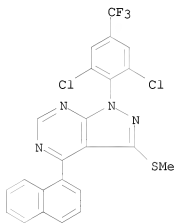
RN 157434-85-0 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[4-(2-chlorophenyl)-3-(methylthio)-1-(2,4,6-trichlorophenyl)-1H-pyrazolo[3,4-d]pyrimidin-6-yl]-, ethyl ester (CA INDEX NAME)



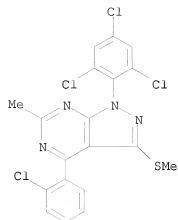
RN 157434-86-1 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-3-(methylthio)-4-(1-naphthalenyl)- (CA INDEX NAME)



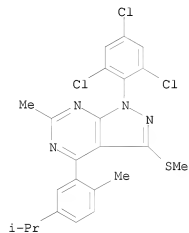
RN 157434-87-2 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(2-chlorophenyl)-6-methyl-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



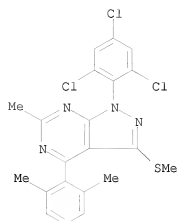
RN 157434-88-3 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-methyl-4-[2-methyl-5-(1-methylethyl)phenyl]-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



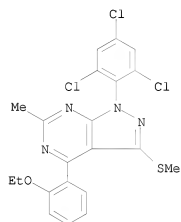
RN 157434-89-4 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(2,6-dimethylphenyl)-6-methyl-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



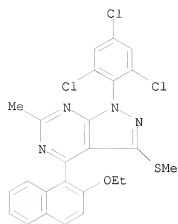
RN 157434-90-7 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(2-ethoxyphenyl)-6-methyl-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



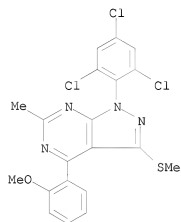
RN 157434-91-8 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(2-ethoxy-1-naphthalenyl)-6-methyl-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



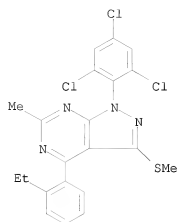
RN 157434-92-9 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(2-methoxyphenyl)-6-methyl-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



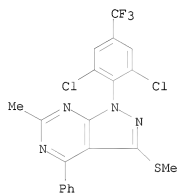
RN 157434-93-0 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(2-ethylphenyl)-6-methyl-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



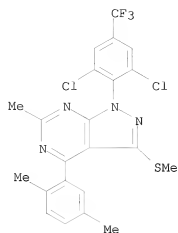
RN 157434-94-1 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-6-methyl-3-(methylthio)-4-phenyl- (CA INDEX NAME)



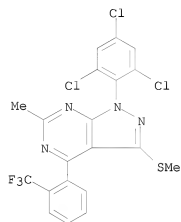
RN 157434-95-2 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(2,5-dimethylphenyl)-6-methyl-3-(methylthio)- (CA INDEX NAME)

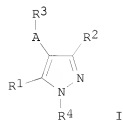


RN 157434-96-3 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-methyl-3-(methylthio)-1-(2,4,6-trichlorophenyl)-4-[2-(trifluoromethyl)phenyl]- (CA INDEX NAME)



GI



AB The title compds. [I; A = CO; A together with the carbons to which they

are attached forms (un)substituted 5-pyridyl; R2 = H, alkyl, OH, etc.; R3 = (un)substituted Ph, naphthyl, 3-8 membered cycloalkyl, etc.; R4 = (un)substituted Ph, naphthyl, 9-12 membered bicycloalkyl] which have corticotropin releasing factor (CRF) antagonist activity and therefore are useful in the treatment of a wide range of diseases including stress-related illnesses, were prepared E.g., a 4-step detailed synthesis of I [A = CO; R1 = NH2; R2 = SMe; R3 = 2,5-Me2C6H3; R4 = 2,6-Cl2-4-F3CC6H2], starting with p-xylene and  $\alpha$ -bromoacetyl chloride, was given. The binding activity for compds. I generally ranges from about 0.2 nM - 10  $\mu$ M.

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT



L14 ANSWER 30 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:659367 CAPLUS

DOCUMENT NUMBER: 131:271888

TITLE: Preparation of nitrogenous heterocyclic compounds for inhibiting phosphorylation of PDGF receptors

INVENTOR(S): Matsuno, Kenji; Nomoto, Yuji; Ichimura, Michio; Ide, Shin-ichi; Oda, Shoji

PATENT ASSIGNEE(S): Kyowa Hakko Kogyo Co., Ltd., Japan

SOURCE: PCI Int. Appl., 96 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 9951582	A1	19991014	WO 1999-JP1665	19990331
W: AU, BG, BR, CA, CN, CZ, HU, ID, IL, IN, JP, KR, MX, NO, NZ, PL, RO, SG, SI, SK, UA, US, VN, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2326324	A1	19991014	CA 1999-2326324	19990331
AU 9930539	A	19991025	AU 1999-30539	19990331
EP 1067123	A1	20010110	EP 1999-912061	19990331
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO				
US 6423716	B1	20020723	US 2000-647490	20000929
PRIORITY APPLN. INFO.:			JP 1998-87514	A 19980331
			WO 1999-JP1665	W 19990331

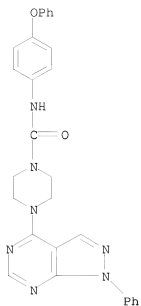
OTHER SOURCE(S): MARPAT 131:271888

IT 245449-38-1P 245449-39-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of nitrogenous heterocyclic compds. for inhibiting phosphorylation of PDGF receptors)

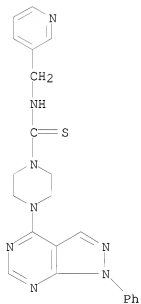
RN 245449-38-1 CAPLUS

CN 1-Piperazinecarboxamide, N-(4-phenoxyphenyl)-4-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)- (CA INDEX NAME)



RN 245449-39-2 CAPLUS

CN 1-Piperazinecarbothioamide, 4-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-N-(3-pyridinylmethyl)-, dihydrochloride (9CI) (CA INDEX NAME)



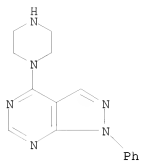
● 2 HCl

IT 245449-98-3P

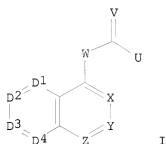
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of nitrogenous heterocyclic compds. for inhibiting phosphorylation of PDGF receptors)

RN 245449-98-3 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-phenyl-4-(1-piperazinyl)- (CA INDEX NAME)



GI



AB Nitrogenous heterocyclic compds. [I; W = 1,4-piperazinediyl, etc.; U = NR1R2 (wherein R1 = H, (un)substituted alkyl, etc.; R2 = H, etc.), OR4 or SR5 (wherein R4, R5 = (un)substituted alkyl, alicyclic alkyl, heterocyclic, etc.); V = O, S, NR6, or CR7R8 (wherein R6 = R1, cyano, OH, NO2, etc.; R7, R8 = H, cyano, NO2, etc.); at least one of X, Y, and Z = N and the remainder are the same or different and each represents N or CRA (wherein RA = R1, halo, cyano, NO2, etc.); and D1, D2, D3, and D4 each independently = N, O, S, CRB (wherein RB = RA), etc. or any adjacent two of D1-D4 in combination = N, O, S, etc.] or pharmacol. acceptable salts thereof, effective in inhibiting phosphorylation of PDGF receptors and in treating cell proliferation diseases such as arteriosclerosis, vascular reocclusion, cancers, glomerulosclerosis, etc., are prepared CF3CO2H was added to a solution of tert-Bu 4-[(4-phenoxyphenyl)carbamoyl]-1-piperazinecarboxylate in CH2Cl2 with stirring under cooling, the concentrate

was

dissolved in DMF containing Et3N and the solution was treated with 6-chloropurine under Ar at room temperature to give 71% N-(4-phenoxyphenyl)-4-(6-purinyl)-1-piperazinecarboxamide, which showed IC50 of 0.29 μM against phosphorylation of PDGF receptor. Four addnl. I showed 66-95% inhibition. Tablet, powder and syrup formulations were given.

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 31 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:295955 CAPLUS

DOCUMENT NUMBER: 131:67655

TITLE: Use of the Suzuki reaction for the synthesis of aryl-substituted heterocycles as corticotropin-releasing hormone (CRH) antagonists

AUTHOR(S): Cocuzza, Anthony J.; Chidester, Dennis R.; Culp, Steven; Fitzgerald, Lawrence; Gilligan, Paul

CORPORATE SOURCE: Chemical and Physical Sciences Department, DuPont Pharmaceuticals Company, Wilmington, DE, 19880-0500, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (1999), 9(7), 1063-1066

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

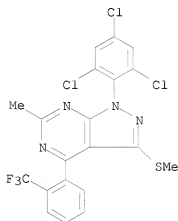
IT 157434-96-3P

RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(aryl-substituted heterocycles as corticotropin-releasing hormone antagonists, and preparation thereof using Suzuki reaction)

RN 157434-96-3 CAPLUS

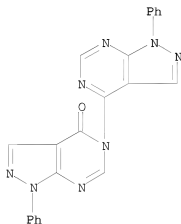
CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-methyl-3-(methylthio)-1-(2,4,6-trichlorophenyl)-4-[2-(trifluoromethyl)phenyl]- (CA INDEX NAME)



AB The Suzuki reaction has been used to synthesize a variety of aryl-substituted heterocyclic antagonists of the CRH1 receptor. Examples with several different heterocyclic cores are potent CRH receptor ligands.

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 32 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1998:187263 CAPLUS  
 DOCUMENT NUMBER: 128:270579  
 TITLE: Several approaches to cyanide ion-catalyzed synthesis of 4-aro-yl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidines  
 AUTHOR(S): Miyashita, Akira; Suzuki, Yumiko; Ohta, Kiyono; Iwamoto, Ken-ichi; Higashino, Takeo  
 CORPORATE SOURCE: Sch. Pharmaceutical Scis., Univ. Shizuoka, Shizuoka, 422, Japan  
 SOURCE: Heterocycles (1998), 47(1), 407-414  
 CODEN: HTCYAM; ISSN: 0385-5414  
 PUBLISHER: Japan Institute of Heterocyclic Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 128:270579  
 IT 66370-43-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (cyanide ion-catalyzed synthesis of aroylphenylpyrazolo[3,4-d]pyrimidines)  
 RN 66370-43-2 CAPLUS  
 CN [4,5'-(4'H)-Bi-1H-pyrazolo[3,4-d]pyrimidin]-4'-one, 1,1'-diphenyl- (CA INDEX NAME)



AB 4-Aroyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidines (I) were formed in low yields by reaction of 4-chloro-1-phenyl-1H-pyrazolo[3,4-d]pyrimidine with arenecarbaldehydes in the presence of potassium cyanide. Similar reaction of 4-tosyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidine with arenecarbaldehydes gave I in higher yields (60-74%). In the presence of catalytic amts. of both sodium p-toluenesulfonate and potassium cyanide, the reaction gave I in good yields.

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 33 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:133890 CAPLUS

DOCUMENT NUMBER: 128:230337

TITLE: Carbon-carbon bond cleavage of  $\alpha$ -hydroxybenzylheteroarenes catalyzed by cyanide ion: retro-benzoin condensation affords ketones and heteroarenes and benzyl migration affords benzylheteroarenes and arenecarbaldehydes

AUTHOR(S): Suzuki, Yumiko; Takemura, Yuki; Iwamoto, Ken-ichi; Higashino, Takeo; Miyashita, Akira

CORPORATE SOURCE: School Pharmaceutical Sciences, Univ. Shizuoka, Shizuoka, 422, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1998), 46(2), 199-206

CODEN: CPBTAL; ISSN: 0009-2363

PUBLISHER: Pharmaceutical Society of Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

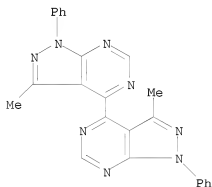
OTHER SOURCE(S): CASREACT 128:230337

IT 204520-33-2P

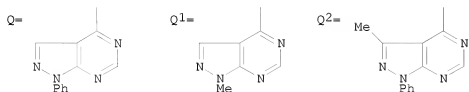
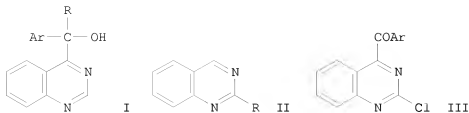
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of ketones, heteroarenes, benzylheteroarenes, and arenecarbaldehydes by retro-benzoin condensation and benzyl migration catalyzed by cyanide ion)

RN 204520-33-2 CAPLUS

CN 4,4'-Bi-1H-pyrazolo[3,4-d]pyrimidine, 3,3'-dimethyl-1,1'-diphenyl- (CA INDEX NAME)



GI



AB 4-( $\alpha$ -Benzyl- $\alpha$ -hydroxybenzyl)quinazoline underwent retro-benzoin condensation catalyzed by cyanide ion to give deoxybenzoin and quinazoline. Similarly, several nitrogen-containing heteroarene, e.g., I (Ar = Ph, 4-ClC<sub>6</sub>H<sub>4</sub>, 4-MeOC<sub>6</sub>H<sub>4</sub>, 2-furyl, 4-BrC<sub>6</sub>H<sub>4</sub>, R = PhCH<sub>2</sub>, Ph, Me) having an  $\alpha$ -hydroxybenzyl group at the  $\alpha$ -position of the nitrogen underwent retro-benzoin type condensation to afford ketones ArCOR and heteroarenes, e.g., 2-phenylquinoxaline. However, similar reaction of pyrazolopyrimidines ArC(OH)Rhet (Ar = Ph, 4-ClC<sub>6</sub>H<sub>4</sub>, 4-MeOC<sub>6</sub>H<sub>4</sub>, R = PhCH<sub>2</sub>, Ph, Me, Het = Q, Q1, Q2) having an  $\alpha$ -benzyl- $\alpha$ -hydroxybenzyl group resulted in benzyl migration, giving benzylpyrazolopyrimidines HetCH<sub>2</sub>Ph and arenecarbaldehydes ArCHO. Tetrabutylammonium cyanide (Bu<sub>4</sub>N<sup>+</sup>CN<sup>-</sup>) was a more effective cyanide ion donor than KCN. The retro-benzoin condensation was applied to the synthesis of 2-substituted quinazolines II [R = MeO, Me<sub>2</sub>N, Cl, 4-BrC<sub>6</sub>H<sub>4</sub>CM<sub>2</sub>(OH)] from 2-chloro-4-aryloxyquinazolines III, using the aroyl group as a protecting and electron-withdrawing group.

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 1995:439538 CAPLUS

DOCUMENT NUMBER: 123:111977

ORIGINAL REFERENCE NO.: 123:20005a,20008a

TITLE: Catalytic action of azolium salts. IV. Preparations of

4-arylquinazolines and 4-aryl-1H-pyrazolo[3,4-d]pyrimidines by catalytic action of 1,3-dimethylimidazolium iodide

AUTHOR(S): Miyashita, Akira; Matsuda, Hideaki; Suzuki, Yumiko; Iwamoto, Ken-ichi; Higashino, Takeo

CORPORATE SOURCE: School Pharmaceutical Sciences, University Shizuoka, Shizuoka, 422, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1994), 42(10), 2017-22

CODEN: CPBTAL; ISSN: 0009-2363

PUBLISHER: Pharmaceutical Society of Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 123:111977

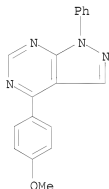
IT 87412-76-8P

RL: BYP (Byproduct); PREP (Preparation)

(azolium salt-catalyzed arylation of chloroquinazolines or chloropyrazolopyrimidines with arenecarboxaldehydes)

RN 87412-76-8 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(4-methoxyphenyl)-1-phenyl- (CA INDEX NAME)



AB The ability of 1,3-dimethylimidazolium iodide (1) to catalyze the arylation of the chloroheteroarenes with arenecarbaldehydes as sources of the aryl groups was examined in order to develop a preparative method of arylheteroarenes. In the presence of 1, the treatment of the 4-chloroquinazolines with arenecarbaldehydes in refluxing THF or dioxane led to the 4-arylquinazolines in excellent yields. Similar reaction of 4-chloro-1H-pyrazolo[3,4-d]pyrimidines with arenecarbaldehydes yielded the corresponding 4-aryl-1H-pyrazolo[3,4-d]pyrimidines. Compound 1 seems to catalyze the arylation with a wider range of arenecarbaldehydes as compared with 1,3-dimethylbenzimidazolium iodide.

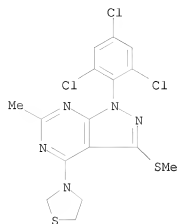


L14 ANSWER 35 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1994:680680 CAPLUS  
 DOCUMENT NUMBER: 121:280680  
 ORIGINAL REFERENCE NO.: 121:51247a,51250a  
 TITLE: Pyrazolo[3,4-d]pyrimidines as ACTH-Releasing Factor Antagonists  
 INVENTOR(S): Chen, Yuhpyng Liang  
 PATENT ASSIGNEE(S): Pfizer Inc., USA  
 SOURCE: PCT Int. Appl., 62 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9413677	A1	19940623	WO 1993-US11333	19931126
W: AU, BR, CA, CZ, JP, KR, NO, NZ, PL, RU, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
TW 444018	B	20010701	TW 1998-87121000	19931122
CA 2150709	A1	19940623	CA 1993-2150709	19931126
CA 2150709	C	19990316		
AU 9457281	A	19940704	AU 1994-57281	19931126
AU 680226	B2	19970724		
EP 674642	A1	19951004	EP 1994-903283	19931126
EP 674642	B1	20000823		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
RU 2124016	C1	19981227	RU 1995-113966	19931126
BR 9307648	A	19990525	BR 1993-7648	19931126
PL 177028	B1	19990930	PL 1993-309359	19931126
AT 195738	T	20000915	AT 1994-903283	19931126
CZ 287319	B6	20001011	CZ 1995-1586	19931126
ES 2150482	T3	20001201	ES 1994-903283	19931126
PT 674642	T	20010131	PT 1994-903283	19931126
IL 107944	A	20001206	IL 1993-107944	19931209
ZA 9309405	A	19950615	ZA 1993-9405	19931215
FI 9305675	A	19940618	FI 1993-5675	19931216
FI 105920	B1	20001031		
CN 1094048	A	19941026	CN 1993-120128	19931216
CN 1034175	B	19970305		
HU 70426	A2	19951030	HU 1993-3613	19931216
HU 221507	B	20021028		
NO 9502399	A	19950816	NO 1995-2399	19950616
US 6218397	B1	20010417	US 1998-148075	19980904
GR 3034507	T3	20001229	GR 2000-402197	20000928
PRIORITY APPLN. INFO.:			US 1992-992229	A 19921217
			WO 1993-US11333	W 19931126
			US 1995-481413	B1 19950615

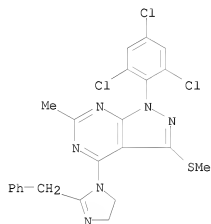
OTHER SOURCE(S): MARPAT 121:280680  
 IT 158949-82-7P 158949-86-1P 158949-87-2P  
 158949-90-7P 158950-45-9P 158950-46-0P  
 158950-47-1P 158950-49-3P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of, as ACTH-releasing factor antagonist)  
 RN 158949-82-7 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-methyl-3-(methylthio)-4-(3-thiazolidinyl)-

1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



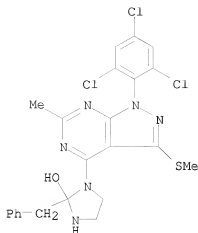
RN 158949-86-1 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[4,5-dihydro-2-(phenylmethyl)-1H-imidazol-1-yl]-6-methyl-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



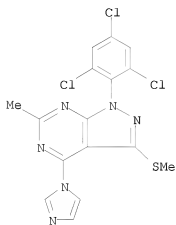
RN 158949-87-2 CAPLUS

CN 2-Imidazolidinol, 1-[6-methyl-3-(methylthio)-1-(2,4,6-trichlorophenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]-2-(phenylmethyl)- (CA INDEX NAME)



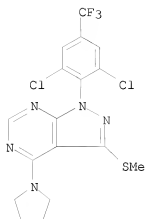
RN 158949-90-7 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(1H-imidazol-1-yl)-6-methyl-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



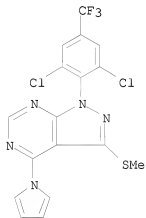
RN 158950-45-9 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-3-(methylthio)-4-(1-pyrrolidinyl)- (CA INDEX NAME)



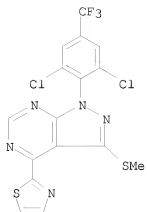
RN 158950-46-0 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-3-(methylthio)-4-(1H-pyrrol-1-yl)- (CA INDEX NAME)



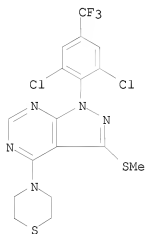
RN 158950-47-1 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-3-(methylthio)-4-(2-thiazolyl)- (CA INDEX NAME)

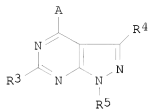


RN 158950-49-3 CAPLUS

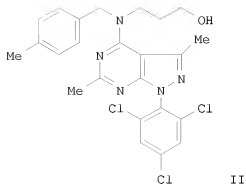
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-3-(methylthio)-4-(4-thiomorpholinyl)- (CA INDEX NAME)



GI



I



II

AB ACTH-releasing factor antagonists I (A = amino group, alkyl alkylthio, etc.; R3, R4 = H, alkyl, halo, etc.; R5 = Ph, naphthyl, heteroaryl, etc.) were disclosed. I are useful in the treatment of illnesses induced or facilitated by CRF, such as inflammatory disorders, and depression and anxiety related disorders. Specifically claimed example compound is 3-[(4-methylbenzyl)[3,6-dimethyl-1-(2,4,6-trichlorophenyl)pyrazolo[4,3-d]pyrimidin-4-yl]amino]-1-propanol (II). Pharmacol. test data for I were not shown.

L14 ANSWER 36 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1994:621999 CAPLUS

DOCUMENT NUMBER: 121:221999

ORIGINAL REFERENCE NO.: 121:40185a,40188a

TITLE: Preparation of adenosine kinase-inhibiting purine nucleoside analogs as antiinflammatory agents

INVENTOR(S): Firestein, Gary Steven; Ugarkar, Bheemarao Ganapatrao; Miller, Leonard Paul; Gruber, Harry Edward; Bullough, David Andrew; Erion, Mark David; Castellino, Angelo John

PATENT ASSIGNEE(S): Gensia, Inc., USA

SOURCE: PCT Int. Appl., 114 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 14

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9417803	A1	19940818	WO 1994-US1340	19940203
W: AT, AU, BB, BG, BR, CA, CH, CN, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, UZ				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9462365	A	19940829	AU 1994-62365	19940203
EP 682519	A1	19951122	EP 1994-909558	19940203
R: CH, DE, FR, GB, IT, LI				
US 5646128	A	19970708	US 1994-349125	19941201
PRIORITY APPLN. INFO.:			US 1993-14190	A 19930203
			US 1989-408707	B2 19890915
			US 1990-466979	B2 19900118
			US 1991-647117	B2 19910123
			US 1991-812916	B2 19911223
			US 1994-192645	B1 19940203
			WO 1994-US1340	W 19940203

OTHER SOURCE(S): MARPAT 121:221999

IT 158077-98-6P

RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use);

BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent);

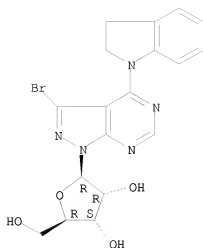
USES (Uses)

(preparation of adenosine kinase-inhibiting purine nucleoside analogs as antiinflammatory agents)

RN 158077-98-6 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 3-bromo-4-(2,3-dihydro-1H-indol-1-yl)-1- $\beta$ -D-ribofuranosyl- (CA INDEX NAME)

Absolute stereochemistry.



IT 144928-51-8P 158077-99-7P 158078-00-3P

158078-01-4P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

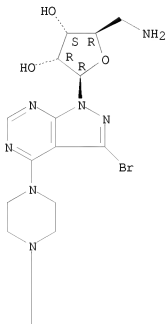
(preparation of adenosine kinase-inhibiting purine nucleoside analogs as antiinflammatory agents)

RN 144928-51-8 CAPLUS

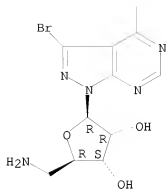
CN 1H-Pyrazolo[3,4-d]pyrimidine, 4,4'-(1,4-piperazinediyl)bis[1-(5-amino-5-deoxy-β-D-ribofuranosyl)-3-bromo-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A





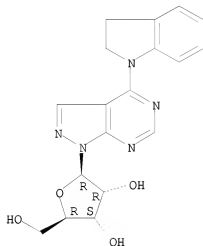


● x HCl

RN 158077-99-7 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(2,3-dihydro-1H-indol-1-yl)-1-β-D-ribofuranosyl- (CA INDEX NAME)

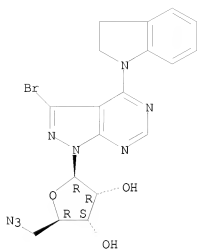
Absolute stereochemistry.



RN 158078-00-3 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-(5-azido-5-deoxy-β-D-ribofuranosyl)-3-bromo-4-(2,3-dihydro-1H-indol-1-yl)- (9CI) (CA INDEX NAME)

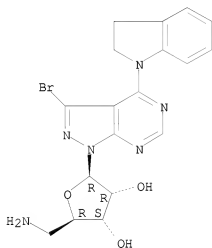
Absolute stereochemistry.



RN 158078-01-4 CAPLUS

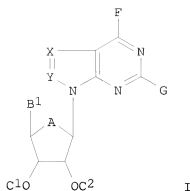
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-(5-amino-5-deoxy-β-D-ribofuranosyl)-3-bromo-4-(2,3-dihydro-1H-indol-1-yl)-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● x HCl

GI



AB Novel nucleosides I [A = O, CH<sub>2</sub>, S; B' = (CH<sub>2</sub>)<sub>n</sub>B, alkenyl, alkynyl; B = H, alkyl, alkoxy, NH<sub>2</sub>, alkylamino, etc.; C1, C2 = H, acyl, hydrocarbyloxycarbonyl, or C1C2 = C(:O), α-alkoxyalkylidene; X = CD; D = H, halo, alkyl, cyano, CO<sub>2</sub>H, etc.; Y = N, CE; E = H, halo, alkyl, alkylthio; F = alkyl, aryl, halo, cyano, indolyl, pyrrolidinyl, etc.; G = H, halo, alkyl, alkoxy, alkylamino, alkylthio; n = 1-4], prepared by multistep procedures which are described, selectively inhibit adenosine kinase and are useful in treatment of conditions characterized by an inflammatory response. Such conditions include sepsis, arthritis, autoimmune disease, burns, psoriasis, conjunctivitis, etc. Thus, mice with endotoxemia resulting from injection of *Escherichia coli* lipopolysaccharide showed a dose-dependent increase in survival in response to i.v. injection of the adenosine kinase inhibitor, 4-amino-1-(5-amino-5-deoxy-1-β-D-ribofuranosyl)-3-bromopyrazolo[3,4-d]pyrimidine-HCl; this effect was antagonized by the adenosine receptor antagonist 8-(p-sulphophenyl)theophylline.

L14 ANSWER 37 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1994:557639 CAPLUS  
 DOCUMENT NUMBER: 121:157639  
 ORIGINAL REFERENCE NO.: 121:28545a,28548a  
 TITLE: Pyrazoles and pyrazolopyrimidines having  
 corticotropin-releasing factor antagonist activity  
 INVENTOR(S): Faraci, William Stephen; Welch, Willard McKowan, Jr.  
 PATENT ASSIGNEE(S): Pfizer Inc., USA  
 SOURCE: PCT Int. Appl., 65 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 3  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9413643	A1	19940623	WO 1993-US10359	19931103
W: AU, BR, CA, CZ, JP, KR, NO, NZ, PL, RU, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2150483	A1	19940623	CA 1993-2150483	19931103
CA 2150483	C	19990914		
CA 2272136	A1	19940623	CA 1993-2272136	19931103
CA 2272136	C	20041207		
CA 2272138	A1	19940623	CA 1993-2272138	19931103
CA 2272138	C	20020305		
AU 9454548	A	19940704	AU 1994-54548	19931103
AU 690527	B2	19980430		
EP 674624	A1	19951004	EP 1993-925103	19931103
EP 674624	B1	19990120		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 07509725	T	19951026	JP 1993-514147	19931103
JP 2862374	B2	19990303		
CZ 284157	B6	19980812	CZ 1995-1585	19931103
AT 175961	T	19990215	AT 1993-925103	19931103
PL 175831	B1	19990226	PL 1993-309356	19931103
ES 2126661	T3	19990401	ES 1993-925103	19931103
BR 9307659	A	19990629	BR 1993-7659	19931103
RU 2142946	C1	19991220	RU 1995-113969	19931103
IL 107946	A	19980924	IL 1993-107946	19931209
HU 67457	A2	19950428	HU 1993-3591	19931215
ZA 9309404	A	19950615	ZA 1993-9404	19931215
FI 9305674	A	19940618	FI 1993-5674	19931216
FI 113648	B1	20040531		
CN 1092768	A	19940928	CN 1993-120120	19931216
CN 1060768	B	20010117		
US 5712303	A	19980127	US 1995-448529	19950614
NO 9502395	A	19950816	NO 1995-2395	19950616
NO 304831	B1	19990222		
MX 9805325	A	20040824	MX 1998-5325	19980629
AU 9878431	A	19981001	AU 1998-78431	19980727
AU 713804	B2	19991209		
NO 9805494	A	19950816	NO 1998-5494	19981125
NO 306111	B1	19990920		
US 20020016333	A1	20020207	US 1999-377350	19990819
US 6441018	B2	20020827		
US 20020049227	A1	20020425	US 1999-377569	19990819
US 6448265	B2	20020910		
PRIORITY APPLN. INFO.:			US 1992-992225	A 19921217

CA 1993-2150483	A3 19931103
WO 1993-US10359	W 19931103
US 1995-448529	A3 19950614
US 1997-961413	A3 19971030
US 1997-961414	A3 19971030

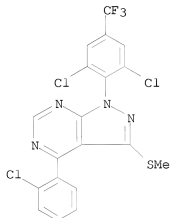
OTHER SOURCE(S): MARPAT 121:157639

IT 157434-80-5P 157434-81-6P 157434-82-7P  
 157434-83-8P 157434-84-9P 157434-85-0P  
 157434-86-1P 157434-87-2P 157434-88-3P  
 157434-89-4P 157434-90-7P 157434-91-8P  
 157434-92-9P 157434-93-0P 157434-94-1P  
 157434-95-2P 157434-96-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of, as ACTH-releasing factor antagonist)

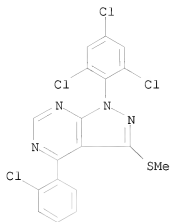
RN 157434-80-5 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(2-chlorophenyl)-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-3-(methylthio)- (CA INDEX NAME)



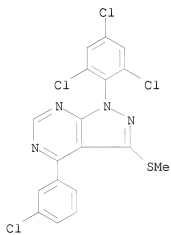
RN 157434-81-6 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(2-chlorophenyl)-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



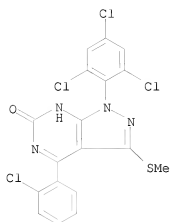
RN 157434-82-7 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(3-chlorophenyl)-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



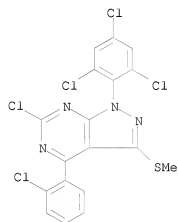
RN 157434-83-8 CAPLUS

CN 6H-Pyrazolo[3,4-d]pyrimidin-6-one, 4-(2-chlorophenyl)-1,5-dihydro-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (9CI) (CA INDEX NAME)



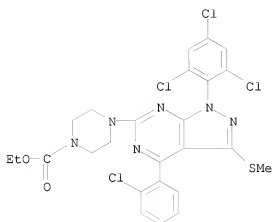
RN 157434-84-9 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-chloro-4-(2-chlorophenyl)-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



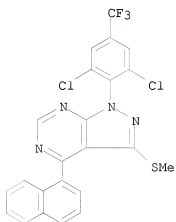
RN 157434-85-0 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[4-(2-chlorophenyl)-3-(methylthio)-1-(2,4,6-trichlorophenyl)-1H-pyrazolo[3,4-d]pyrimidin-6-yl]-, ethyl ester (CA INDEX NAME)



RN 157434-86-1 CAPLUS

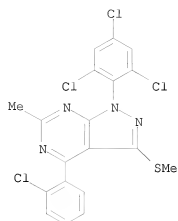
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-3-(methylthio)-4-(1-naphthalenyl)- (CA INDEX NAME)



RN 157434-87-2 CAPLUS

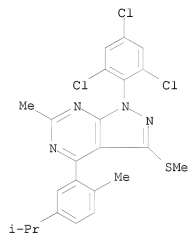
CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(2-chlorophenyl)-6-methyl-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)





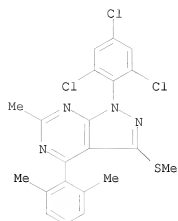
RN 157434-88-3 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-methyl-4-[2-methyl-5-(1-methylethyl)phenyl]-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



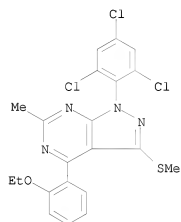
RN 157434-89-4 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(2,6-dimethylphenyl)-6-methyl-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



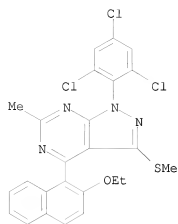
RN 157434-90-7 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(2-ethoxyphenyl)-6-methyl-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



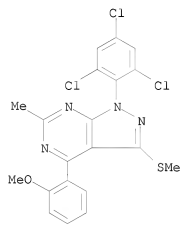
RN 157434-91-8 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(2-ethoxy-1-naphthalenyl)-6-methyl-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



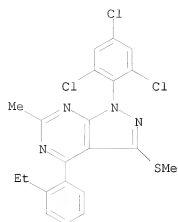
RN 157434-92-9 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(2-methoxyphenyl)-6-methyl-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



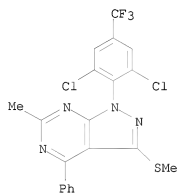
RN 157434-93-0 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(2-ethylphenyl)-6-methyl-3-(methylthio)-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



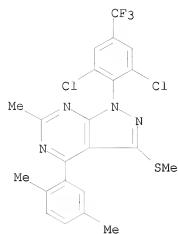
RN 157434-94-1 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-6-methyl-3-(methylthio)-4-phenyl- (CA INDEX NAME)



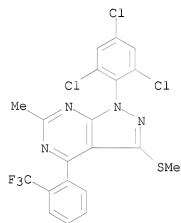
RN 157434-95-2 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(2,5-dimethylphenyl)-6-methyl-3-(methylthio)- (CA INDEX NAME)

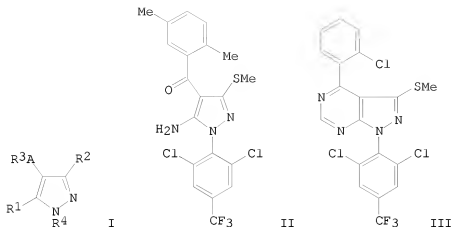


RN 157434-96-3 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-methyl-3-(methylthio)-1-(2,4,6-trichlorophenyl)-4-[2-(trifluoromethyl)phenyl]- (CA INDEX NAME)

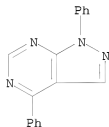


GI

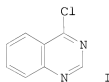


AB Pyrazoles and pyrazolopyrimidines I (R1H, alkyl, amino, etc.; R2 = H, alkyl, alkoxy, etc.; R3, R4 = Ph, naphthyl, thenyl, etc.; A = CO, SO2; AR1 = pyrimidinyl or pyridinyl group) were disclosed. I have ACTH releasing factor antagonist activity. As such, they are effective in the treatment of a wide range of diseases including stress-related illnesses, such as depression, headaches, inflammatory disorders, fertility disorders, etc. Prepared example compds. are 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(2,5-dimethylbenzoyl)-3-(methylthio)pyrazole (II) and 4-(2-chlorophenyl)-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-3-(methylthio)pyrazolo[3,4]pyrimidine (III).

L14 ANSWER 38 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1994:482648 CAPLUS  
 DOCUMENT NUMBER: 121:82648  
 ORIGINAL REFERENCE NO.: 121:14837a,14840a  
 TITLE: Ring opening of 4-chloroquinazoline into  
 2-arylmethyleneaminobenzonitrile by Grignard reaction  
 AUTHOR(S): Miyashita, Akira; Sasaki, Takami; Oishi, Etsuo;  
 Higashino, Takeo  
 CORPORATE SOURCE: Sch. Pharm. Sci., Univ. Shizuoka, Shizuoka, 422, Japan  
 SOURCE: Heterocycles (1994), 37(2), 823-31  
 CODEN: HETCYAM; ISSN: 0385-5414  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 121:82648  
 IT 53645-78-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 53645-78-6 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 1,4-diphenyl- (CA INDEX NAME)



GI



AB The treatment of 4-chloroquinazoline (I) with arylmagnesium bromide (e.g., PhMgBr) in THF resulted in the formation of 2-arylmethyleneaminobenzonitrile (II, e.g., PhCH:NC<sub>6</sub>H<sub>4</sub>CN-2 ). Continued reaction of ring opening of I and subsequent hydrolysis of the products (II) afforded the corresponding arenecarbaldehydes (e.g., PhCHO) + 2-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CN.

L14 ANSWER 39 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1993:234420 CAPLUS  
DOCUMENT NUMBER: 118:234420  
ORIGINAL REFERENCE NO.: 118:40623a, 40626a  
TITLE: Adenosine kinase inhibitors  
INVENTOR(S): Browne, Clinton E.; Ugarkar, Bheemarao G.; Mullane, Kevin M.; Gruber, Harry E.; Bullough, David A.; Erion, Mark D.; Castellino, Angelo  
PATENT ASSIGNEE(S): Gensia Pharmaceuticals, Inc., USA  
SOURCE: Eur. Pat. Appl., 87 pp.  
CODEN: EPXXDW  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 14  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 496617	A1	19920729	EP 1992-300580	19920123
EP 496617	B1	19991201		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, PT, SE				
CA 2100863	A1	19920724	CA 1992-2100863	19920121
WO 9212718	A1	19920806	WO 1992-US515	19920121
W: AU, CA, FI, NO				
AU 9213599	A	19920827	AU 1992-13599	19920121
AU 665184	B2	19951221		
JP 05112595	A	19930507	JP 1992-10094	19920123
IL 100742	A	19960618	IL 1992-100742	19920123
AT 187175	T	19991215	AT 1992-300580	19920123
NO 9302628	A	19930923	NO 1993-2628	19930721
NO 180418	B	19970106		
NO 180418	C	19970416		
US 5646128	A	19970708	US 1994-349125	19941201
PRIORITY APPLN. INFO.:			US 1991-647117	A 19910123
			US 1991-812916	A 19911223
			US 1989-408707	B2 19890915
			US 1990-466979	B2 19900118
			WO 1992-US515	W 19920121
			US 1993-14190	B2 19930203
			US 1994-192645	B1 19940203

OTHER SOURCE(S): MARPAT 118:234420

IT 144928-46-1P

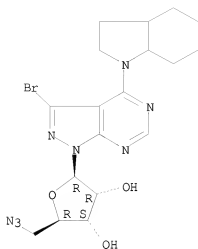
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and reduction of)

RN 144928-46-1 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-(5-azido-5-deoxy- $\beta$ -D-ribofuranosyl)-3-bromo-4-(octahydro-1H-indol-1-yl)- (9CI) (CA INDEX NAME)

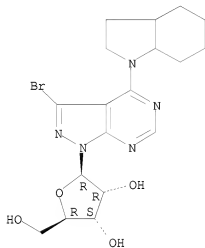
Absolute stereochemistry.





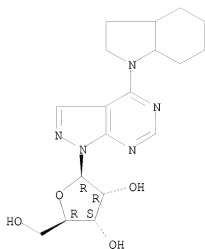
IT 144928-34-7P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and reductive debromination of)  
 RN 144928-34-7 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 3-bromo-4-(octahydro-1H-indol-1-yl)-1-β-  
 D-ribofuranosyl- (CA INDEX NAME)

Absolute stereochemistry.



IT 144928-36-9P 144928-49-4P 144928-51-8P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 144928-36-9 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(octahydro-1H-indol-1-yl)-1-β-D-  
 ribofuranosyl- (CA INDEX NAME)

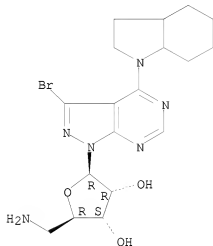
Absolute stereochemistry.



RN 144928-49-4 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-(5-amino-5-deoxy- $\beta$ -D-ribofuranosyl)-3-bromo-4-(octahydro-1H-indol-1-yl)-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



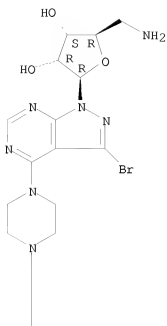
● x HCl

RN 144928-51-8 CAPLUS

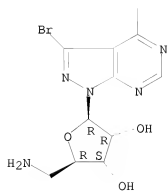
CN 1H-Pyrazolo[3,4-d]pyrimidine, 4,4'-(1,4-piperazinediyl)bis[1-(5-amino-5-deoxy- $\beta$ -D-ribofuranosyl)-3-bromo-], hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

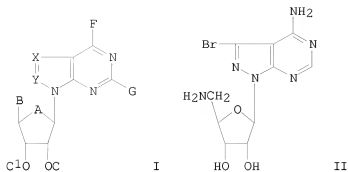


PAGE 2-A



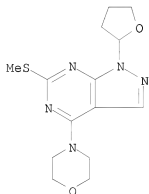
● x HCl

GI

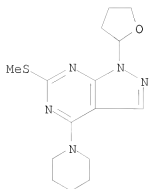


AB Nucleoside analogs I [A = O, CH<sub>2</sub>, S; B = (un)substituted C1-4 alkyl; C, Cl = H, protective group(s); X = (un)substituted CH; Y = N, (un)substituted CH; F = alkyl, aryl, aralkyl, halogen, (un)substituted NH<sub>2</sub>, substituted OH or SH, cyano, cyanoalkyl; G = H, halogen, alkyl, alkoxy, alkylamino, alkylthio] were prepared. Thus, the analog II was prepared from the pyrimidinone via the azide. II has an adenosine kinase-inhibiting ED<sub>50</sub> of <10 nM and was effective in improving post-ischemic functional recovery in isolated guinea pig heart and in preclin. angina models.

L14 ANSWER 40 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1991:156594 CAPLUS  
 DOCUMENT NUMBER: 114:156594  
 ORIGINAL REFERENCE NO.: 114:26259a,26262a  
 TITLE: QSAR study on the antiviral activity of  
 2,6,9-substituted purines and related analogs  
 AUTHOR(S): Prabhakar, Y. S.; Bhakuni, D. S.  
 CORPORATE SOURCE: Med. Chem. Div., Cent. Drug Res. Inst., Lucknow, 226  
 001, India  
 SOURCE: Indian Journal of Biochemistry & Biophysics (1990),  
 27(5), 342-7  
 CODEN: IJBBBQ; ISSN: 0301-1208  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 IT 112697-19-5 112697-21-9 112697-22-0  
 112697-23-1 112697-27-5 112697-29-7  
 112697-30-0 112697-31-1 112697-34-4  
 112697-36-6 112697-37-7 112697-38-8  
 115523-23-4 115523-24-5 115523-30-3  
 115523-31-4 115523-36-9 115523-37-0  
 115538-43-7  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
 study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES  
 (Uses)  
 (antiviral activity of, QSAR study of)  
 RN 112697-19-5 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-(methylthio)-4-(4-morpholinyl)-1-  
 (tetrahydro-2-furanyl)- (CA INDEX NAME)

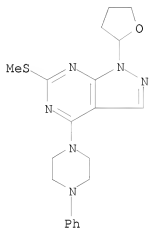


RN 112697-21-9 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-(methylthio)-4-(1-piperidinyl)-1-  
 (tetrahydro-2-furanyl)- (CA INDEX NAME)



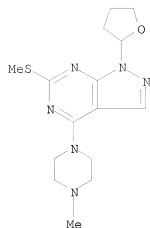
RN 112697-22-0 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-(methylthio)-4-(4-phenyl-1-piperazinyl)-1-(tetrahydro-2-furanyl)- (CA INDEX NAME)



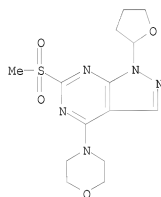
RN 112697-23-1 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(4-methyl-1-piperazinyl)-6-(methylthio)-1-(tetrahydro-2-furanyl)- (CA INDEX NAME)



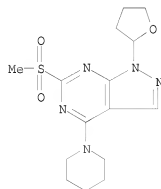
RN 112697-27-5 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-(methylsulfonyl)-4-(4-morpholinyl)-1-(tetrahydro-2-furanyl)- (CA INDEX NAME)



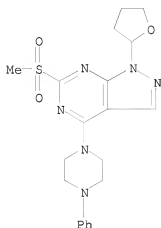
RN 112697-29-7 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-(methylsulfonyl)-4-(1-piperidinyl)-1-(tetrahydro-2-furanyl)- (CA INDEX NAME)



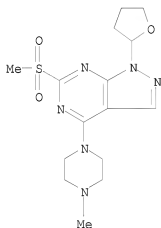
RN 112697-30-0 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-(methylsulfonyl)-4-(4-phenyl-1-piperazinyl)-1-(tetrahydro-2-furanyl)- (CA INDEX NAME)



RN 112697-31-1 CAPLUS

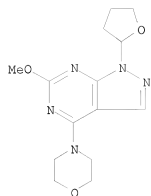
CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(4-methyl-1-piperazinyl)-6-(methylsulfonyl)-1-(tetrahydro-2-furanyl)- (CA INDEX NAME)



RN 112697-34-4 CAPLUS

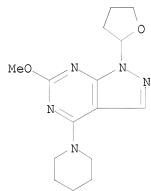
CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-methoxy-4-(4-morpholinyl)-1-(tetrahydro-2-furanyl)- (CA INDEX NAME)





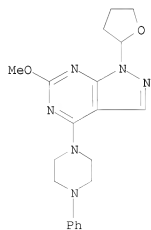
RN 112697-36-6 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-methoxy-4-(1-piperidinyl)-1-(tetrahydro-2-furanyl)- (CA INDEX NAME)



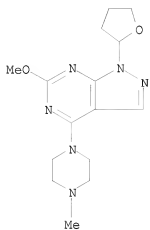
RN 112697-37-7 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-methoxy-4-(4-phenyl-1-piperazinyl)-1-(tetrahydro-2-furanyl)- (CA INDEX NAME)



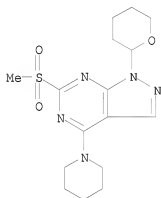
RN 112697-38-8 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-methoxy-4-(4-methyl-1-piperazinyl)-1-(tetrahydro-2-furanyl)- (CA INDEX NAME)



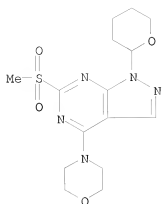
RN 115523-23-4 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-(methylsulfonyl)-4-(1-piperidinyl)-1-(tetrahydro-2H-pyran-2-yl)- (CA INDEX NAME)



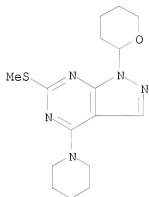
RN 115523-24-5 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-(methylsulfonyl)-4-(4-morpholinyl)-1-(tetrahydro-2H-pyran-2-yl)- (CA INDEX NAME)



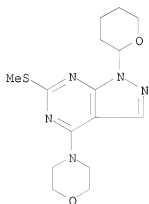
RN 115523-30-3 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-(methylthio)-4-(1-piperidinyl)-1-(tetrahydro-2H-pyran-2-yl)- (CA INDEX NAME)



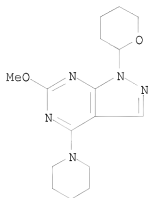
RN 115523-31-4 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-(methylthio)-2-(4-morpholinyl)-1-(tetrahydro-2H-pyran-2-yl)- (9CI) (CA INDEX NAME)



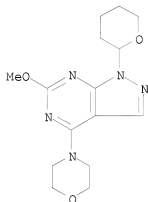
RN 115523-36-9 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-methoxy-4-(1-piperidinyl)-1-(tetrahydro-2H-pyran-2-yl)- (CA INDEX NAME)



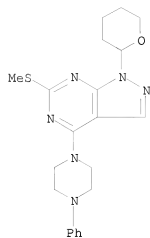
RN 115523-37-0 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-methoxy-4-(4-morpholinyl)-1-(tetrahydro-2H-pyran-2-yl)- (CA INDEX NAME)

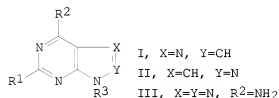


RN 115538-43-7 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-(methylthio)-4-(4-phenyl-1-piperazinyl)-1-(tetrahydro-2H-pyran-2-yl)- (CA INDEX NAME)

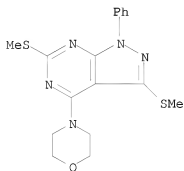


GI

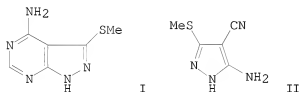


AB A QSAR study was carried out on the antiviral activity of 2,6,9-substituted purines [I, R<sub>1</sub> = e.g., OH, NH<sub>2</sub>, OMe, Cl, OEt, R<sub>2</sub> = alkylamino, piperidinyl, acyloxycarbonylalkylthio, or OH, R<sub>3</sub> = 1-(β-D-ribofuranosyl) or tetrahydropyranyl], 2,4,6-substituted pyrazolo[3,4-d]pyrimidines (II, R<sub>1</sub> = e.g., SMe, SO<sub>2</sub>Me, OMe, R<sub>2</sub> = NH<sub>2</sub>, NHMe, morpholinyl, R<sub>3</sub> = 2-tetrahydrofuran-2-yl and 6-amino-2,9-substituted 8-azaadenines [III, R<sub>1</sub> = SEt, SPr, SBu, and R<sub>3</sub> = H or 1-(β-D-ribofuranosyl)] by using hydrophobicity, van der Waals volume and indicator parameters as descriptors. Optimum hydrophobicity and structural requirements were identified for each prototype.

L14 ANSWER 41 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1990:611929 CAPLUS  
 DOCUMENT NUMBER: 113:211929  
 ORIGINAL REFERENCE NO.: 113:35811a,35814a  
 TITLE: Synthesis of pyrazolo[3,4-d]pyrimidine derivatives  
 using ketene dithioacetals  
 AUTHOR(S): Tominaga, Yoshinori; Honkawa, Yasumasa; Hara, Mayumi;  
 Hosomi, Akira  
 CORPORATE SOURCE: Fac. Pharm. Sci., Nagasaki Univ., Nagasaki, 852, Japan  
 SOURCE: Journal of Heterocyclic Chemistry (1990), 27(3),  
 775-83  
 CODEN: JHTCAD; ISSN: 0022-152X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 113:211929  
 IT 130224-63-4P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 130224-63-4 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 3,6-bis(methylthio)-4-(4-morpholinyl)-1-  
 phenyl- (CA INDEX NAME)



GI



AB The cyclization of 5-amino-3-methylthiopyrazole-4-carbonitriles or  
 4-carboxamides, which were prepared by the reaction of ketene dithioacetals  
 [bis(methylthio)methylenemalononitrile, bis(methylthio)methylenecyanoaceta  
 mide] with hydrazines (hydrazine hydrate, phenylhydrazine,  
 p-chlorophenylhydrazine, p-nitrophenylhydrazine), with formamide or carbon  
 disulfide proceeded to give the corresponding 4-amino- or  
 4-hydroxy-3-methylthiopyrazolo[3,4-d]pyrimidines in good yields.  
 3-Aminopyrazolo[3,4-d]pyrimidine derivs. were also obtained by the  
 application of the cyclization reaction of 3,5-diaminopyrazoles with  
 formamide. E.g., pyrazolopyrimidine I was obtained in 72% yield from

aminopyrazolecarbonitrile II with HCONH<sub>2</sub>.

L14 ANSWER 42 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:440551 CAPLUS

DOCUMENT NUMBER: 113:40551

ORIGINAL REFERENCE NO.: 113:6891a,6894a

TITLE: Studies on pyrazolo[3,4-d]pyrimidine derivatives.  
XVII. Reactions of 5-benzoyl-4,5-dihydro-6-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidine-4-carbonitrile (the 6-methylpyrazolopyrimidine Reissert compound)

AUTHOR(S): Miyashita, Akira; Sato, Susumu; Taido, Naokata; Tanji, Kenichi; Oishi, Etsuo; Higashino, Takeo

CORPORATE SOURCE: Sch. Pharm. Sci., Univ. Shizuoka, Shizuoka, 422, Japan  
SOURCE: Chemical & Pharmaceutical Bulletin (1990), 38(1), 230-3

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

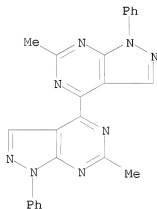
OTHER SOURCE(S): CASREACT 113:40551

IT 128039-01-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

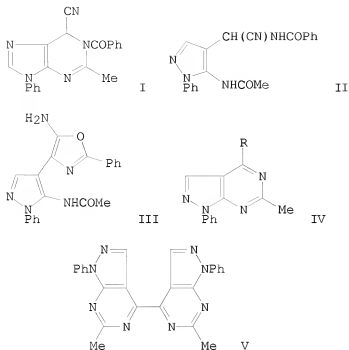
RN 128039-01-0 CAPLUS

CN 4,4'-Bi-1H-pyrazolo[3,4-d]pyrimidine, 6,6'-dimethyl-1,1'-diphenyl- (CA  
INDEX NAME)



GI





AB Acid hydrolysis of the 6-methylpyrazolopyrimidine Reissert compound I gave the ring-opened product II and the oxazole III. Alkaline hydrolysis of I afforded the 6-methylpyrazolopyrimidine IV (R = H) and benzoic acid. The anion of I underwent both aromatization and rearrangement, resulting in the formation of IV (R = H, CN, PhCO<sub>2</sub>, PhCO<sub>2</sub>CHPh), the dimer V, and PhCO<sub>2</sub>CHPhCOPh. The addition reaction of the anion of I with aldehydes was also examined

L14 ANSWER 43 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1988:473841 CAPLUS

DOCUMENT NUMBER: 109:73841

ORIGINAL REFERENCE NO.: 109:12385a,12388a

TITLE: Nucleosides. Part XVIII. Synthesis of 6-methoxy/methylthio-4-N-substituted-1-(2'-tetrahydropyranyl/2'-hydroxyethoxymethyl)-1H-pyrazolo[3,4-d]pyrimidines and their biological activity

AUTHOR(S): Deo, K.; Avasthi, K.; Pratap, Ram; Kar, K.; Bhakuni, D. S.

CORPORATE SOURCE: Cent. Drug Res. Inst., Lucknow, 226 001, India  
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1987), 26B(10), 963-7

DOCUMENT TYPE: Journal

LANGUAGE: English

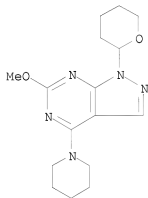
OTHER SOURCE(S): CASREACT 109:73841

IT 115523-36-9P 115523-37-0P 115538-43-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and virucidal and antiallergic activity of)

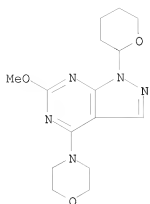
RN 115523-36-9 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-methoxy-4-(1-piperidinyl)-1-(tetrahydro-2H-pyran-2-yl)- (CA INDEX NAME)



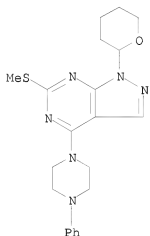
RN 115523-37-0 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-methoxy-4-(4-morpholinyl)-1-(tetrahydro-2H-pyran-2-yl)- (CA INDEX NAME)



RN 115538-43-7 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-(methylthio)-4-(4-phenyl-1-piperazinyl)-1-(tetrahydro-2H-pyran-2-yl)- (CA INDEX NAME)

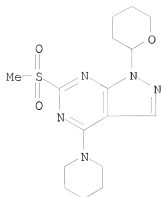


IT 115523-23-4P 115523-24-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation, methoxylation, and virucidal activity of)

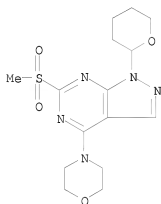
RN 115523-23-4 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-(methylsulfonyl)-4-(1-piperidinyl)-1-(tetrahydro-2H-pyran-2-yl)- (CA INDEX NAME)



RN 115523-24-5 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-(methylsulfonyl)-4-(4-morpholinyl)-1-(tetrahydro-2H-pyran-2-yl)- (CA INDEX NAME)

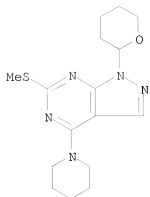


IT 115523-30-3P 115523-31-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation, oxidation, and virucidal antiallergic activity of)

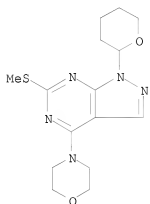
RN 115523-30-3 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-(methylthio)-4-(1-piperidinyl)-1-(tetrahydro-2H-pyran-2-yl)- (CA INDEX NAME)

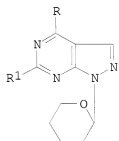


RN 115523-31-4 CAPLUS

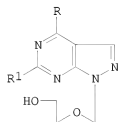
CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-(methylthio)-2-(4-morpholinyl)-1-(tetrahydro-2H-pyran-2-yl)- (9CI) (CA INDEX NAME)



GI



I



II

AB 6-Methylthio-4-amino 1-(2-tetrahydropyranyl)-1H-pyrazolo[3,4-d]pyrimidines (I, R = NHNH<sub>2</sub>, NH<sub>2</sub>, substituted amino, R<sub>1</sub> = SMe), the corresponding sulfones I (R<sub>1</sub> = SO<sub>2</sub>Me), 6-methoxypyrazolo[3,4-d]pyrimidines I (R<sub>1</sub> = OMe)

and the 1-(2-hydroxyethoxymethyl)pyrazolo[3,4-d]pyrimidines II (R = NH<sub>2</sub>, R<sub>1</sub> = SMe, OMe) have been synthesized. I (R<sub>1</sub> = SMe, OMe) show significant passive cutaneous anaphylaxis activity. I (R = piperidino, R<sub>1</sub> = SO<sub>2</sub>Me) and II (R = NHAc, R<sub>1</sub> = SO<sub>2</sub>Me) exhibit 80 and 90% inhibition resp. against the Ranikhet disease virus (RDV).

L14 ANSWER 44 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1988:454727 CAPLUS

DOCUMENT NUMBER: 109:54727

ORIGINAL REFERENCE NO.: 109:9230h,9231a

TITLE: Studies on pyrazolo[3,4-d]pyrimidine derivatives. XV.  
Reactions involving the formation of the anion of the  
Reissert compound derived from 1H-pyrazolo[3,4-  
d]pyrimidine

AUTHOR(S): Higashino, Takeo; Sato, Susumu; Miyashita, Akira;  
Katori, Tatsuhiko

CORPORATE SOURCE: Sch. Pharm. Sci., Univ. Shizuoka, Shizuoka, 422, Japan  
SOURCE: Chemical & Pharmaceutical Bulletin (1987), 35(10),  
4078-86

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

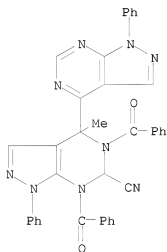
OTHER SOURCE(S): CASREACT 109:54727

IT 115393-20-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and hydrolysis of)

RN 115393-20-9 CAPLUS

CN [4,4'-Bi-1H-pyrazolo[3,4-d]pyrimidine]-6-carbonitrile,  
5,7-dibenzoyl-4,5,6,7-tetrahydro-4-methyl-1,1'-diphenyl- (CA INDEX NAME)

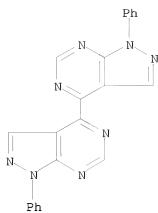


IT 59563-52-9P 115393-19-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

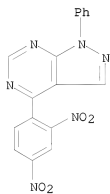
RN 59563-52-9 CAPLUS

CN 4,4'-Bi-1H-pyrazolo[3,4-d]pyrimidine, 1,1'-diphenyl- (CA INDEX NAME)



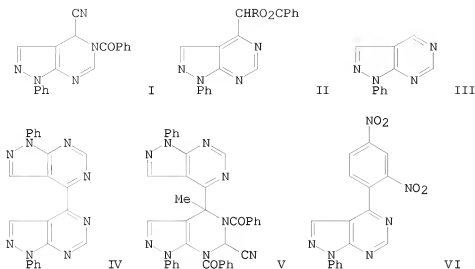
RN 115393-19-6 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(2,4-dinitrophenyl)-1-phenyl- (CA INDEX NAME)



GI





AB The anion of benzoylcyanodihydropyrazolopyrimidine I reacted with RCHO (R = heptyl, Me<sub>2</sub>CH, Ph, 4-MeC<sub>6</sub>H<sub>4</sub>, 4-MeOC<sub>6</sub>H<sub>4</sub>, 4-ClC<sub>6</sub>H<sub>4</sub>, 2-MeC<sub>6</sub>H<sub>4</sub>, 2-MeOC<sub>6</sub>H<sub>4</sub>, 2-ClC<sub>6</sub>H<sub>4</sub>) to give pyrazolopyrimidinyl benzoates II and products derived from the decomposition of I, e.g., phenypyrazolopyrimidine III, bis[phenylprazolopyrimidine] IV, RCOCHRO<sub>2</sub>CPh and RCH(CN)O<sub>2</sub>CPh (R = same as above). The anion of I reacted with MeI and 2,4-(O<sub>2</sub>N)C<sub>6</sub>H<sub>3</sub>Cl to give methylation and arylation products V and VI resp., however, with other electrophiles only the decomposition products were obtained.

L14 ANSWER 45 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1988:75765 CAPLUS

DOCUMENT NUMBER: 108:75765

ORIGINAL REFERENCE NO.: 108:12555a,12558a

TITLE: Studies in nucleosides. Part XV. Synthesis of 6-methoxy/methylthio-4-N-substituted-1-(2-tetrahydrofuran-1-yl)-1H-pyrazolo[3,4-d]pyrimidines and their biological activity

AUTHOR(S): Hasan, Ahmad; Pratap, Ram; Joshi, M. N.; Kar, K.; Bhakuni, D. S.

CORPORATE SOURCE: Cent. Drug Res. Inst., Lucknow, 226 001, India

SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1987), 26B(3), 284-6

CODEN: IJSBDB; ISSN: 0376-4699

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 108:75765

IT 112697-19-5P 112697-21-9P 112697-22-0P

112697-23-1P 112697-27-5P 112697-29-7P

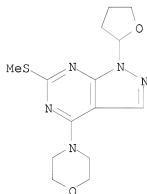
112697-30-0P 112697-31-1P 112697-34-4P

112697-36-6P 112697-37-7P 112697-38-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (preparation and biol. activity of)

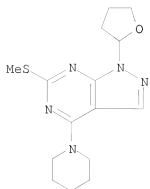
RN 112697-19-5 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-(methylthio)-4-(4-morpholinyl)-1-(tetrahydro-2-furanyl)- (CA INDEX NAME)



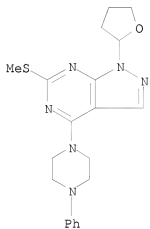
RN 112697-21-9 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-(methylthio)-4-(1-piperidinyl)-1-(tetrahydro-2-furanyl)- (CA INDEX NAME)



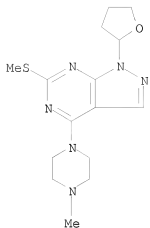
RN 112697-22-0 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-(methylthio)-4-(4-phenyl-1-piperazinyl)-1-(tetrahydro-2-furanyl)- (CA INDEX NAME)



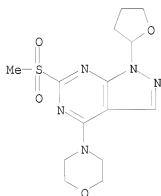
RN 112697-23-1 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(4-methyl-1-piperazinyl)-6-(methylthio)-1-(tetrahydro-2-furanyl)- (CA INDEX NAME)



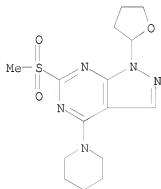
RN 112697-27-5 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-(methylsulfonyl)-4-(4-morpholinyl)-1-(tetrahydro-2-furanyl)- (CA INDEX NAME)



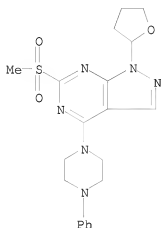
RN 112697-29-7 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-(methylsulfonyl)-4-(1-piperidinyl)-1-(tetrahydro-2-furanyl)- (CA INDEX NAME)



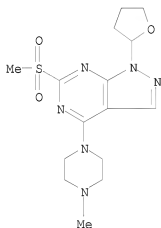
RN 112697-30-0 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-(methylsulfonyl)-4-(4-phenyl-1-piperazinyl)-1-(tetrahydro-2-furanyl)- (CA INDEX NAME)



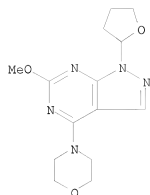
RN 112697-31-1 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(4-methyl-1-piperazinyl)-6-(methylsulfonyl)-1-(tetrahydro-2-furanyl)- (CA INDEX NAME)



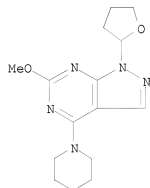
RN 112697-34-4 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-methoxy-4-(4-morpholinyl)-1-(tetrahydro-2-furanyl)- (CA INDEX NAME)



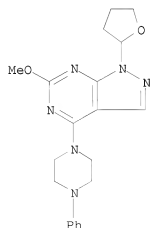
RN 112697-36-6 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-methoxy-4-(1-piperidinyl)-1-(tetrahydro-2-furanyl)- (CA INDEX NAME)



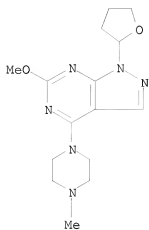
RN 112697-37-7 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-methoxy-4-(4-phenyl-1-piperazinyl)-1-(tetrahydro-2-furanyl)- (CA INDEX NAME)

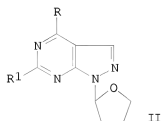
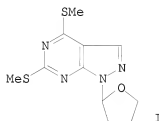


RN 112697-38-8 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-methoxy-4-(4-methyl-1-piperazinyl)-1-(tetrahydro-2-furanyl)- (CA INDEX NAME)

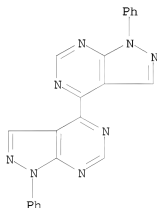


GI

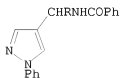
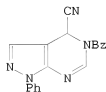


AB Condensation of 4,6-bis(methylthio)pyrazolo[3,4-d]pyrimidine with dihydrofuran in AcOEt in the presence of p-MeC<sub>6</sub>H<sub>4</sub>SO<sub>3</sub>H gave 80% tetrahydrofuran derivative I, which on heating with amines gave the amino derivs. (II; R = NH<sub>2</sub>, MeNH, morpholino, piperidino, etc.; R<sub>1</sub> = MeS; 8 compds.; 43-77% yield), which on oxidation with m-ClC<sub>6</sub>H<sub>4</sub>CO<sub>3</sub>H gave 28-90% II (R same, R<sub>1</sub> = MeSO<sub>2</sub>), which on treatment with NaOMe in MeOH gave 24-52% II (R same, R<sub>1</sub> = MeO). II were evaluated for antiallergic and antiviral activities. II (R = MeNH, piperidino, R<sub>1</sub> = MeSO<sub>2</sub>; R = piperidino, R<sub>1</sub> = MeO) exhibited 100% inhibition against Ranikhet disease virus in vitro.

L14 ANSWER 46 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1987:515553 CAPLUS  
 DOCUMENT NUMBER: 107:115553  
 ORIGINAL REFERENCE NO.: 107:18730h,18731a  
 TITLE: Studies on pyrazolo[3,4-d]pyrimidine derivatives.  
 XIV. Preparation and reactions of  
 1-phenyl-1H-pyrazolo[3,4-d]pyrimidine Reissert  
 compound  
 AUTHOR(S): Higashino, Takeo; Sato, Susumu; Miyashita, Akira;  
 Katori, Tatsuhiko  
 CORPORATE SOURCE: Shizuoka Coll. Pharm., Shizuoka, 422, Japan  
 SOURCE: Chemical & Pharmaceutical Bulletin (1986), 34(11),  
 4569-76  
 CODEN: CPBTAL; ISSN: 0009-2363  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 107:115553  
 IT 59563-52-9P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 59563-52-9 CAPLUS  
 CN 4,4'-Bi-1H-pyrazolo[3,4-d]pyrimidine, 1,1'-diphenyl- (CA INDEX NAME)



GI



AB The Reissert reaction of pyrazolopyrimidine I using BzCl and Me3SiCN and a catalytic amount of AlCl3 gave 95% of the Reissert compound II. Alkaline hydrolysis of II gave I, PhCO2H, and the 4,4'-dimer of I. Acid hydrolysis of II in DMSO proceeded with ring fission to give pyrazoles III (R = cyano, CONH2) and in MeOH to give III (R = cyano, CONH2, CO2Me).





L14 ANSWER 47 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1987:458981 CAPLUS

DOCUMENT NUMBER: 107:58981

ORIGINAL REFERENCE NO.: 107:9797a,9800a

TITLE: Conversion of 4-amino-1H-1,5-benzodiazepine-3-carbonitrile to pyrazolo[3,4-d]pyrimidines, pyrimido[1,6-a]benzimidazole, and pyrazolo[3',4':4,5]pyrimido[1,6-a]benzimidazoles  
Okamoto, Yoshihisa; Togo, Isao; Kurasawa, Yoshihisa; Takagi, Kaname

AUTHOR(S): Sch. Pharm. Sci., Kitasato Univ., Tokyo, 108, Japan

CORPORATE SOURCE: Journal of Heterocyclic Chemistry (1986), 23(6), 1829-31

SOURCE: CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal

LANGUAGE: English

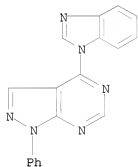
OTHER SOURCE(S): CASREACT 107:58981

IT 109385-63-9P 109385-64-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

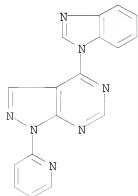
RN 109385-63-9 CAPLUS

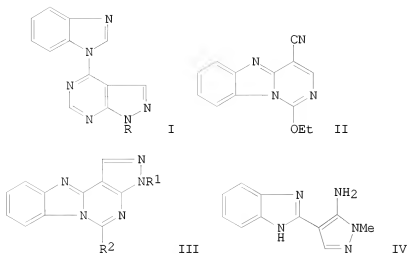
CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(1H-benzimidazol-1-yl)-1-phenyl- (CA INDEX NAME)



RN 109385-64-0 CAPLUS

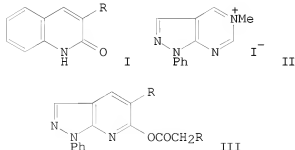
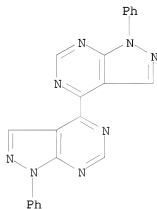
CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(1H-benzimidazol-1-yl)-1-(2-pyridinyl)-  
(CA INDEX NAME)





AB Pyrazolopyrimidines I (R = Me, Ph, 2-pyridyl), pyrimidobenzimidazole II, and pyrazolopyrimidinobenzimidazoles III (R1 = Me, Ph; R2 = H, Me, Et) were prepared from compds. which were readily obtained from 4-amino-1H-1,5-benzodiazepine-3-carbonitrile. E.g., refluxing aminopyrazolylbenzimidazole IV with HC(OEt), for 1 h gave 92% III (R1 = Me, R2 = H).

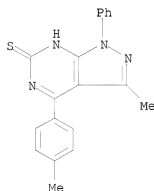
L14 ANSWER 48 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1987:458971 CAPLUS  
 DOCUMENT NUMBER: 107:58971  
 ORIGINAL REFERENCE NO.: 107:9793a,9796a  
 TITLE: Transformation of quinazoline into 2(1H)-quinolinones  
 with alkanolic anhydrides  
 AUTHOR(S): Higashino, Takeo; Goto, Ayako; Miyashita, Akira;  
 Hayashi, Eisaku  
 CORPORATE SOURCE: Shizuoka Coll. Pharm., Shizuoka, 422, Japan  
 SOURCE: Chemical & Pharmaceutical Bulletin (1986), 34(10),  
 4352-5  
 CODEN: CPBTAL; ISSN: 0009-2363  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 107:58971  
 IT 59563-52-9P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 59563-52-9 CAPLUS  
 CN 4,4'-Bi-1H-pyrazolo[3,4-d]pyrimidine, 1,1'-diphenyl- (CA INDEX NAME)



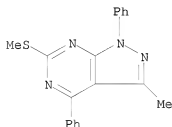
AB Quinazoline was transformed into 3-substituted 2(1H)-quinolinones I by

reaction with alkanolic anhydrides  $(RCH_2CO)_2O$  ( $R=H, Me, Et$ ). Similar transformation was also occurred with 5-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidinium iodide II, giving 5-substituted 1-phenyl-1H-pyrazolo[3,4-b]pyridine-6-yl alkanoates III.

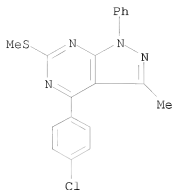
ACCESSION NUMBER: 1987:138379 CAPLUS  
 DOCUMENT NUMBER: 106:138379  
 ORIGINAL REFERENCE NO.: 106:22581a,22584a  
 TITLE: Synthesis and some reactions of 3-methyl-4-aryl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidine-6-thiols  
 AUTHOR(S): Metwally, Saoud A.; Younes, Mansour I.; Metwally, M. A.  
 CORPORATE SOURCE: Fac. Sci., Assiut Univ., Assiut, Egypt  
 SOURCE: Croatica Chemica Acta (1986), 59(2), 483-9  
 CODEN: CCACAA; ISSN: 0011-1643  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 106:138379  
 IT 106924-34-9P 106924-35-0P 106924-36-1P  
 106924-37-2P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and reaction of, with hydrazine)  
 RN 106924-34-9 CAPLUS  
 CN 6H-Pyrazolo[3,4-d]pyrimidine-6-thione, 1,5-dihydro-3-methyl-4-(4-methylphenyl)-1-phenyl- (9CI) (CA INDEX NAME)



RN 106924-35-0 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 3-methyl-6-(methylthio)-1,4-diphenyl- (CA INDEX NAME)

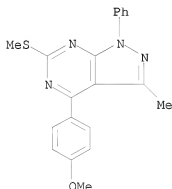


RN 106924-36-1 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(4-chlorophenyl)-3-methyl-6-(methylthio)-1-phenyl- (CA INDEX NAME)



RN 106924-37-2 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(4-methoxyphenyl)-3-methyl-6-(methylthio)-1-phenyl- (CA INDEX NAME)



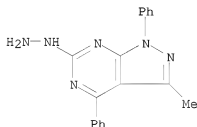
IT 106924-42-9 106924-43-0 106924-44-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation interaction of, with nitrous acid, tetrazolo derivative from)

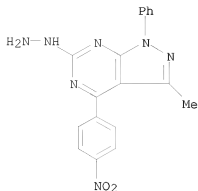
RN 106924-42-9 CAPLUS

CN 6H-Pyrazolo[3,4-d]pyrimidin-6-one, 1,5-dihydro-3-methyl-1,4-diphenyl-, hydrazone (9CI) (CA INDEX NAME)



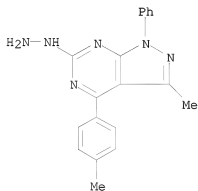
RN 106924-43-0 CAPLUS

CN 6H-Pyrazolo[3,4-d]pyrimidin-6-one, 1,5-dihydro-3-methyl-4-(4-nitrophenyl)-1-phenyl-, hydrazone (9CI) (CA INDEX NAME)



RN 106924-44-1 CAPLUS

CN 6H-Pyrazolo[3,4-d]pyrimidin-6-one, 1,5-dihydro-3-methyl-4-(4-methylphenyl)-1-phenyl-, hydrazone (9CI) (CA INDEX NAME)

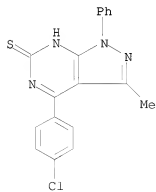


IT 106924-32-7P 106924-33-8P 106936-09-8P  
106936-10-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation, methylation and reaction of, with anisidine)

RN 106924-32-7 CAPLUS

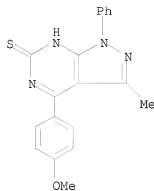
CN 6H-Pyrazolo[3,4-d]pyrimidine-6-thione, 4-(4-chlorophenyl)-1,5-dihydro-3-methyl-1-phenyl- (9CI) (CA INDEX NAME)





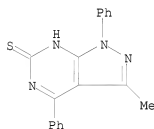
RN 106924-33-8 CAPLUS

CN 6H-Pyrazolo[3,4-d]pyrimidine-6-thione, 1,5-dihydro-4-(4-methoxyphenyl)-3-methyl-1-phenyl- (9CI) (CA INDEX NAME)



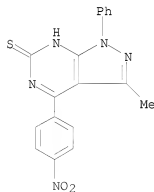
RN 106936-09-8 CAPLUS

CN 6H-Pyrazolo[3,4-d]pyrimidine-6-thione, 1,5-dihydro-3-methyl-1,4-diphenyl- (9CI) (CA INDEX NAME)



RN 106936-10-1 CAPLUS

CN 6H-Pyrazolo[3,4-d]pyrimidine-6-thione, 1,5-dihydro-3-methyl-4-(4-nitrophenyl)-1-phenyl- (9CI) (CA INDEX NAME)

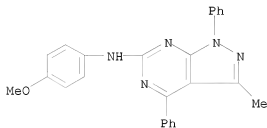


IT 106924-38-3 106924-39-4 106924-40-7  
106924-41-8

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with arylidenepyrimidinethiols)

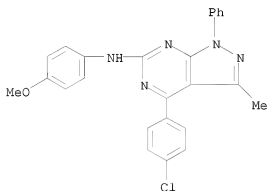
RN 106924-38-3 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidin-6-amine, N-(4-methoxyphenyl)-3-methyl-1,4-diphenyl- (CA INDEX NAME)



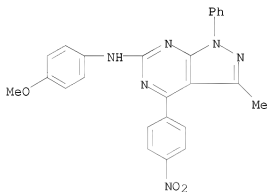
RN 106924-39-4 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidin-6-amine, 4-(4-chlorophenyl)-N-(4-methoxyphenyl)-3-methyl-1-phenyl- (CA INDEX NAME)



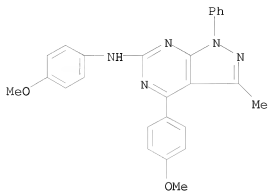
RN 106924-40-7 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidin-6-amine, N-(4-methoxyphenyl)-3-methyl-4-(4-nitrophenyl)-1-phenyl- (CA INDEX NAME)

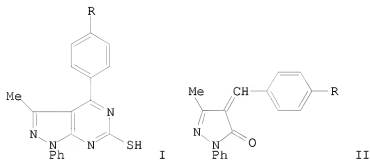


RN 106924-41-8 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidin-6-amine, N,4-bis(4-methoxyphenyl)-3-methyl-1-phenyl- (CA INDEX NAME)

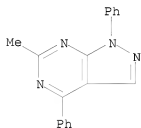


GI



AB The title compds. I (R = H, Me, MeO, Cl, NO<sub>2</sub>) were synthesized by the reaction of thiourea with methylphenylarylidene pyrazolinones II in EtOH containing KOH. The mechanism of this reaction is discussed and further transformation of the products with different reagents (S-methylation, substitution of SH-group by arylamines, hydrazine, and azide) was carried out.

L14 ANSWER 50 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1987:138377 CAPLUS  
 DOCUMENT NUMBER: 106:138377  
 ORIGINAL REFERENCE NO.: 106:22581a,22584a  
 TITLE: Synthesis of quinazolines  
 AUTHOR(S): Bergman, Jan; Brynolf, Anna; Elman, Bjoern; Vuorinen, Eino  
 CORPORATE SOURCE: Dep. Org. Chem., R. Inst. Technol., Stockholm, S-100 44, Swed.  
 SOURCE: Tetrahedron (1986), 42(13), 3697-706  
 CODEN: TETRA; ISSN: 0040-4020  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 106:138377  
 IT 107312-92-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)  
 RN 107312-92-5 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-methyl-1,4-diphenyl- (CA INDEX NAME)



AB Reaction of RMgX (R = Me, Et, Ph, 4-MeC<sub>6</sub>H<sub>4</sub>, Me<sub>2</sub>CH, Bu; X = Cl, Br, iodo) with 2-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CN gave the intermediate 2-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CR:N- (I), which were cyclized to quinazolines by reaction with carbonyl compds. (e.g., acid chlorides, anhydrides, formates, and oxalates). Reaction of I with aldehydes, e.g. PhCHO, gave 1,2-dihydroquinazolines, which were readily dehydrogenated. Reaction of I with ClCO<sub>2</sub>Me gave 4-phenyl-2-quinazolinone, which was reduced to 3,4-dihydro-4-phenyl-2-quinazolinone by NaBH<sub>4</sub> in AcOH.

ACCESSION NUMBER: 1987:102220 CAPLUS

DOCUMENT NUMBER: 106:102220

ORIGINAL REFERENCE NO.: 106:16747a,16750a

TITLE: Synthesis and some reactions of 3-methyl-4-aryl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidine-6-thiols

AUTHOR(S): Metwally, Saoud A.; Younes, Mansour I.

CORPORATE SOURCE: Fac. Sci., Assiut Univ., Assiut, Egypt

SOURCE: Phosphorus and Sulfur and the Related Elements (1986), 27(3), 355-60

CODEN: PREEDF; ISSN: 0308-664X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 106:102220

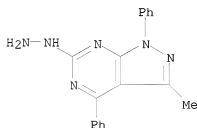
IT 106924-42-9P 106924-43-0P 106924-44-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with nitrous acid, tetrazolopyrazolopyrimidine from)

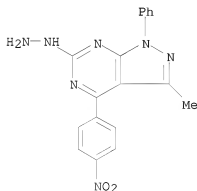
RN 106924-42-9 CAPLUS

CN 6H-Pyrazolo[3,4-d]pyrimidin-6-one, 1,5-dihydro-3-methyl-1,4-diphenyl-, hydrazone (9CI) (CA INDEX NAME)



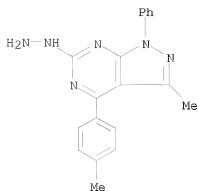
RN 106924-43-0 CAPLUS

CN 6H-Pyrazolo[3,4-d]pyrimidin-6-one, 1,5-dihydro-3-methyl-4-(4-nitrophenyl)-1-phenyl-, hydrazone (9CI) (CA INDEX NAME)



RN 106924-44-1 CAPLUS

CN 6H-Pyrazolo[3,4-d]pyrimidin-6-one, 1,5-dihydro-3-methyl-4-(4-methylphenyl)-1-phenyl-, hydrazone (9CI) (CA INDEX NAME)

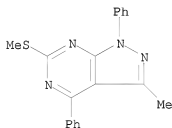


IT 106924-35-0P 106924-36-1P 106924-37-2P  
 106924-38-3P 106924-39-4P 106924-40-7P  
 106924-41-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

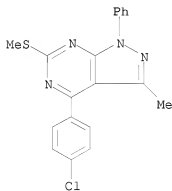
RN 106924-35-0 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 3-methyl-6-(methylthio)-1,4-diphenyl- (CA  
 INDEX NAME)



RN 106924-36-1 CAPLUS

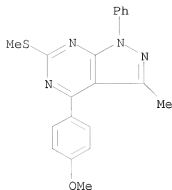
CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(4-chlorophenyl)-3-methyl-6-(methylthio)-1-  
 phenyl- (CA INDEX NAME)



RN 106924-37-2 CAPLUS

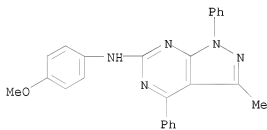
CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(4-methoxyphenyl)-3-methyl-6-(methylthio)-

1-phenyl- (CA INDEX NAME)



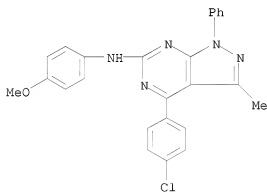
RN 106924-38-3 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidin-6-amine, N-(4-methoxyphenyl)-3-methyl-1,4-diphenyl- (CA INDEX NAME)



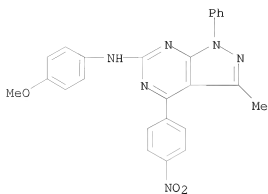
RN 106924-39-4 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidin-6-amine, 4-(4-chlorophenyl)-N-(4-methoxyphenyl)-3-methyl-1-phenyl- (CA INDEX NAME)



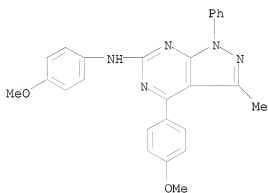
RN 106924-40-7 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidin-6-amine, N-(4-methoxyphenyl)-3-methyl-4-(4-nitrophenyl)-1-phenyl- (CA INDEX NAME)



RN 106924-41-8 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidin-6-amine, N,4-bis(4-methoxyphenyl)-3-methyl-1-phenyl- (CA INDEX NAME)



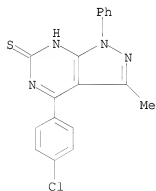
IT 106924-32-7P 106924-33-8P 106924-34-9P

106936-09-8P 106936-10-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation, methylation and amination of)

RN 106924-32-7 CAPLUS

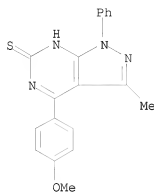
CN 6H-Pyrazolo[3,4-d]pyrimidin-6-thione, 4-(4-chlorophenyl)-1,5-dihydro-3-methyl-1-phenyl- (9CI) (CA INDEX NAME)





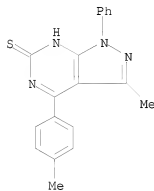
RN 106924-33-8 CAPLUS

CN 6H-Pyrazolo[3,4-d]pyrimidine-6-thione, 1,5-dihydro-4-(4-methoxyphenyl)-3-methyl-1-phenyl- (9CI) (CA INDEX NAME)



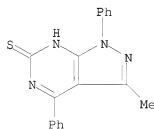
RN 106924-34-9 CAPLUS

CN 6H-Pyrazolo[3,4-d]pyrimidine-6-thione, 1,5-dihydro-3-methyl-4-(4-methylphenyl)-1-phenyl- (9CI) (CA INDEX NAME)



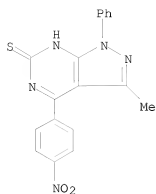
RN 106936-09-8 CAPLUS

CN 6H-Pyrazolo[3,4-d]pyrimidine-6-thione, 1,5-dihydro-3-methyl-1,4-diphenyl- (9CI) (CA INDEX NAME)

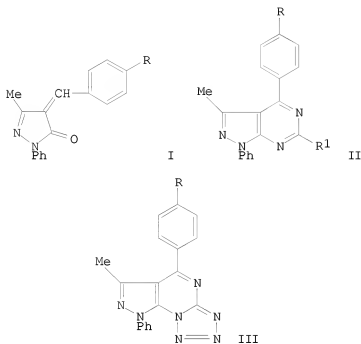


RN 106936-10-1 CAPLUS

CN 6H-Pyrazolo[3,4-d]pyrimidine-6-thione, 1,5-dihydro-3-methyl-4-(4-nitrophenyl)-1-phenyl- (9CI) (CA INDEX NAME)



GI



AB Cyclocondensation of pyrazolinones I (R = H, Cl, NO<sub>2</sub>, OMe, Me) with thiourea in ethanolic KOH gave pyrazolopyrimidines II (R<sub>1</sub> = SH) in 62-93% yields. Amination of II (R<sub>1</sub> = SH) by R<sub>2</sub>NH<sub>2</sub> (R<sub>2</sub> = 4-MeOC<sub>6</sub>H<sub>4</sub>, NH<sub>2</sub>) gave II (R<sub>1</sub> = NHR<sub>2</sub>) in 22-81% yields. Reaction of II (R = H, NO<sub>2</sub>; R<sub>1</sub> = NHNH<sub>2</sub>) with HNO<sub>2</sub> gave tetrazolopyrimidines III in 55-62% yields.

ACCESSION NUMBER: 1985:541908 CAPLUS

DOCUMENT NUMBER: 103:141908

ORIGINAL REFERENCE NO.: 103:22727a,22730a

TITLE: Reactions of the anion of quinazoline Reissert compound (3-benzoyl-3,4-dihydro-4-quinazolinecarbonitrile) with electrophiles  
 AUTHOR(S): Higashino, Takeo; Kokubo, Hiroyasu; Hayashi, Eisaku  
 CORPORATE SOURCE: Shizuoka Coll. Pharm., Shizuoka, 422, Japan  
 SOURCE: Chemical & Pharmaceutical Bulletin (1985), 33(3), 950-61

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

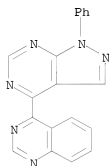
OTHER SOURCE(S): CASREACT 103:141908

IT 98512-46-0P

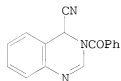
RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 98512-46-0 CAPLUS

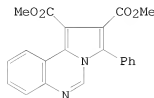
CN Quinazoline, 4-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)- (CA INDEX NAME)



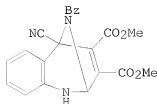
GI



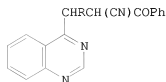
I



II



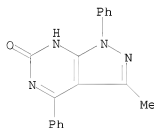
III



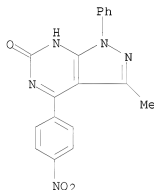
IV

AB Reactions of the quinazoline Reissert compound I with various electrophiles in the presence of NaH in DMF were investigated. The reactions with aldehydes and ketones gave  $\alpha$ -aryl (or alkyl)- and  $\alpha$ -alkyl- $\alpha$ -aryl (or alkyl)-4-quinazolinylmethyl benzoates, resp. The reaction with  $\pi$ -deficient heteroaroms. gave 4-heteroarylquinazolines. Alkylation (or arylation) with alkyl (or aryl) halides gave 4-substituted 3-benzoyl-3,4-dihydro-4-quinazolinecarbonitriles. The reaction with MeO2CC.tplbond.CC(=O)Me gave quinazoline II and ethenoquinazoline III. The reaction with RCH:CHCN (R = H, Me) gave quinazolinyl alkanenitriles IV.

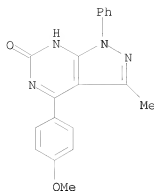
ACCESSION NUMBER: 1985:168303 CAPLUS  
 DOCUMENT NUMBER: 102:168303  
 ORIGINAL REFERENCE NO.: 102:26481a,26484a  
 TITLE: Synthesis, spectral behavior and biological activity of pyrazolo-pyrimidine cyanine dyes  
 AUTHOR(S): El-Maghraby, M. A.; Koraïem, A. I. M.; Abd El-Latif, F. M. E.  
 CORPORATE SOURCE: Chem. Dep., Fac. Sci., Aswan, Egypt  
 SOURCE: Journal of Chemical Technology and Biotechnology, Chemical Technology (1985), 35A(2), 63-72  
 CODEN: JCTTDW; ISSN: 0264-3413  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 IT 55360-99-1 96160-28-0 96183-01-6  
 RL: USES (Uses)  
 (condensation with methyl-substituted heterocyclic base ethiodides and oxidation of)  
 RN 55360-99-1 CAPLUS  
 CN 6H-Pyrazolo[3,4-d]pyrimidin-6-one, 1,7-dihydro-3-methyl-1,4-diphenyl- (CA INDEX NAME)



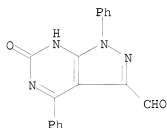
RN 96160-28-0 CAPLUS  
 CN 6H-Pyrazolo[3,4-d]pyrimidin-6-one, 1,5-dihydro-3-methyl-4-(4-nitrophenyl)-1-phenyl- (9CI) (CA INDEX NAME)



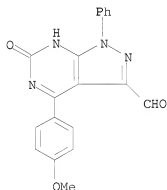
RN 96183-01-6 CAPLUS  
 CN 6H-Pyrazolo[3,4-d]pyrimidin-6-one, 1,5-dihydro-4-(4-methoxyphenyl)-3-methyl-1-phenyl- (9CI) (CA INDEX NAME)



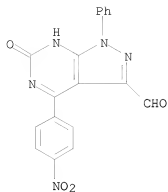
IT 96160-36-0P 96160-37-1P 96160-38-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and condensation with methyl-substituted heterocyclic base  
 ethioides)  
 RN 96160-36-0 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine-3-carboxaldehyde, 5,6-dihydro-6-oxo-1,4-  
 diphenyl- (9CI) (CA INDEX NAME)



RN 96160-37-1 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine-3-carboxaldehyde, 5,6-dihydro-4-(4-  
 methoxyphenyl)-6-oxo-1-phenyl- (9CI) (CA INDEX NAME)



RN 96160-38-2 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine-3-carboxaldehyde, 5,6-dihydro-4-(4-  
 nitrophenyl)-6-oxo-1-phenyl- (9CI) (CA INDEX NAME)



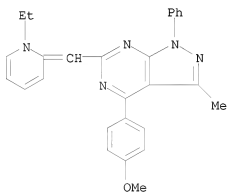
IT 96160-22-4P 96160-24-6P 96160-25-7P

96160-27-9P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and spectra of)

RN 96160-22-4 CAPLUS

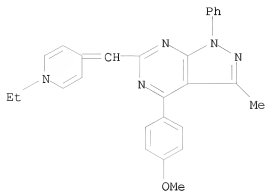
CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-[(1-ethyl-2(1H)-pyridinylidene)methyl]-4-(4-methoxyphenyl)-3-methyl-1-phenyl-, monohydriodide (9CI) (CA INDEX NAME)



● HI

RN 96160-24-6 CAPLUS

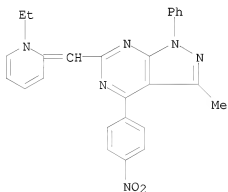
CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-[(1-ethyl-4(1H)-pyridinylidene)methyl]-4-(4-methoxyphenyl)-3-methyl-1-phenyl-, monohydriodide (9CI) (CA INDEX NAME)



● HI

RN 96160-25-7 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-[(1-ethyl-2(1H)-pyridinylidene)methyl]-3-methyl-4-(4-nitrophenyl)-1-phenyl-, monohydriodide (9CI) (CA INDEX NAME)

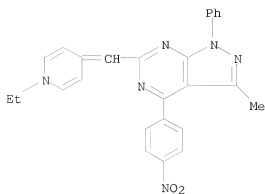


● HI

RN 96160-27-9 CAPLUS

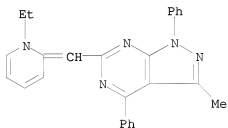
CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-[(1-ethyl-4(1H)-pyridinylidene)methyl]-3-methyl-4-(4-nitrophenyl)-1-phenyl-, monohydriodide (9CI) (CA INDEX NAME)





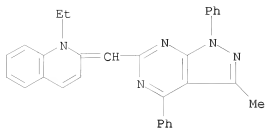
● HI

IT 96160-19-9P 96160-20-2P 96160-21-3P  
 96160-23-5P 96160-26-8P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation, biol. activity and spectra of)  
 RN 96160-19-9 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-[(1-ethyl-2(1H)-pyridinylidene)methyl]-3-methyl-1,4-diphenyl-, monohydriodide (9CI) (CA INDEX NAME)



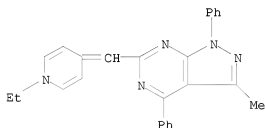
● HI

RN 96160-20-2 CAPLUS  
 CN Quinoline, 1-ethyl-1,2-dihydro-2-[(3-methyl-1,4-diphenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl)methylene]-, monohydriodide (9CI) (CA INDEX NAME)



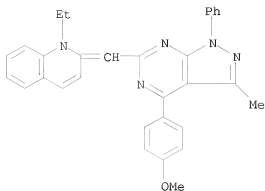
● HI

RN 96160-21-3 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-[(1-ethyl-4(1H)-pyridinylidene)methyl]-3-methyl-1,4-diphenyl-, monohydriodide (9CI) (CA INDEX NAME)



● HI

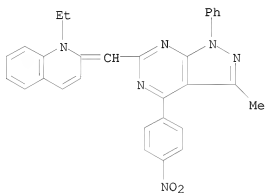
RN 96160-23-5 CAPLUS  
 CN Quinoline, 1-ethyl-1,2-dihydro-2-[[4-(4-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]methylene]-, monohydriodide (9CI) (CA INDEX NAME)



● HI

RN 96160-26-8 CAPLUS

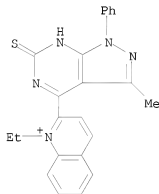
CN Quinoline, 1-ethyl-1,2-dihydro-2-[[3-methyl-4-(4-nitrophenyl)-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]methylene]-, monohydriodide (9CI) (CA INDEX NAME)



● HI

AB New asym. 2(4)-monomethine cyanine dyes, monomethine bases, dicationic cyanines, and styryl cyanines incorporating N-phenyl-1H-pyrazolo[3,4-d]saturated or unsatd. pyrimidine were prepared. The dyes were identified by spectral determination. Bactericidal and fungicidal activity of selected cyanines were tested against bacterial and fungal strains.

L14 ANSWER 54 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1985:80260 CAPLUS  
 DOCUMENT NUMBER: 102:80260  
 ORIGINAL REFERENCE NO.: 102:12595a,12598a  
 TITLE: Apocyanine dyes from 4,5-dioxo-3-methyl-1-phenylpyrazoline  
 AUTHOR(S): Koraïem, Ahmed Ibrahim Mahmoud  
 CORPORATE SOURCE: Chem. Dep., Fac. Sci., Aswan, Egypt  
 SOURCE: Journal fuer Praktische Chemie (Leipzig) (1984), 326(5), 811-16  
 CODEN: JPCEAO; ISSN: 0021-8383  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 102:80260  
 IT 94724-78-4P  
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation, biol. activity and UV absorption of)  
 RN 94724-78-4 CAPLUS  
 CN Quinolinium, 2-(5,6-dihydro-3-methyl-1-phenyl-6-thioxo-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-1-ethyl-, iodide (9CI) (CA INDEX NAME)



● I<sup>-</sup>

GI For diagram(s), see printed CA Issue.  
 AB The title compound [881-05-0] is condensed with  $\alpha$ -picoline-EtI [19760-15-7], quinaldine-EtI [606-55-3], or 2-methylbenzoxazole-EtI [5260-37-7] to form the monomethine derivative which is then brominated and finally cyclocondensed with hydrazines or hydroxylamine to give I (X = NAc, O; A = pyridine, quinoline, benzoxazole ring) or with thiourea to give II. UV-visible absorption data for I and II are reported. I and II in which A = quinoline show bactericidal and fungicidal activity.

L14 ANSWER 55 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1984:156563 CAPLUS

DOCUMENT NUMBER: 100:156563

ORIGINAL REFERENCE NO.: 100:23851a,23854a

TITLE: Studies on pyrazolo[3,4-d]pyrimidine derivatives.  
XIII. Aryl migration of 4-aryl-1H-pyrazolo[3,4-d]pyrimidines to 4-aryl-4,5-dihydro-1H-pyrazolo[3,4-d]pyrimidine-4-carboxylic acids

AUTHOR(S): Higashino, Takeo; Matsushita, Yasuhiko; Takemoto, Masumi; Hayashi, Eisaku

CORPORATE SOURCE: Shizuoka Coll. Pharm., Shizuoka, 422, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1983), 31(11), 3951-8

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 100:156563

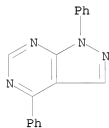
IT 53645-78-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and oxidation of)

RN 53645-78-6 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1,4-diphenyl- (CA INDEX NAME)



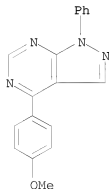
IT 87412-76-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and ring cleavage of)

RN 87412-76-8 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(4-methoxyphenyl)-1-phenyl- (CA INDEX NAME)

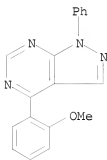


IT 87412-75-7P 87412-78-0P 87412-79-1P  
89549-65-5P 89549-66-6P 89549-67-7P  
89549-86-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

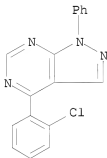
RN 87412-75-7 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(2-methoxyphenyl)-1-phenyl- (CA INDEX  
NAME)



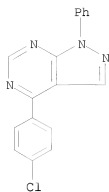
RN 87412-78-0 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(2-chlorophenyl)-1-phenyl- (CA INDEX  
NAME)



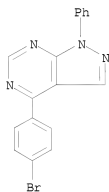
RN 87412-79-1 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(4-chlorophenyl)-1-phenyl- (CA INDEX  
NAME)



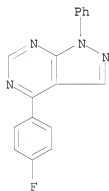
RN 89549-65-5 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(4-bromophenyl)-1-phenyl- (CA INDEX NAME)



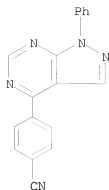
RN 89549-66-6 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(4-fluorophenyl)-1-phenyl- (CA INDEX NAME)



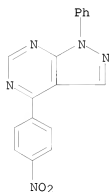
RN 89549-67-7 CAPLUS

CN Benzonitrile, 4-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)- (CA INDEX NAME)

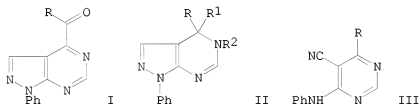


RN 89549-86-0 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(4-nitrophenyl)-1-phenyl- (CA INDEX NAME)



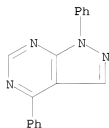
GI



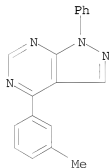
AB Treating pyrazolopyrimidines I (R = Ph, 2-, 4-MeOC6H4, 2-, 4-ClC6H4, 4-BrC6H4, 4-FC6H4, 4-NCC6H4) with NaOH in Me2SO gave pyrazolopyrimidines II (R1 = CO2H, R2 = H) which were oxidized with K3Fe(CN)6 to II (R1R2 = bond). Treating II (R = Ph, 4-MeOC6H4, 4-O2NC6H4, Me; R1R2 = bond) with NaOH in Me2SO gave the corresponding pyrimidinecarbonitriles III.



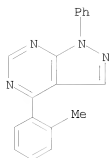
L14 ANSWER 56 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1983:612496 CAPLUS  
 DOCUMENT NUMBER: 99:212496  
 ORIGINAL REFERENCE NO.: 99:32703a,32706a  
 TITLE: Aryl coupling reactions of pyrazolo[3,4-d]pyrimidin-4-yl radicals  
 AUTHOR(S): Press, Jeffery B.; Eudy, Nancy H.; Morton, George O.  
 CORPORATE SOURCE: Lederle Lab., Am. Cyanamid Co., Pearl River, NY, 10965, USA  
 SOURCE: Journal of Organic Chemistry (1983), 48(24), 4605-11  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 99:212496  
 IT 53645-78-6P 87412-72-4P 87412-73-5P  
 87412-74-6P 87412-75-7P 87412-76-8P  
 87412-77-9P 87412-78-0P 87412-79-1P  
 87412-80-4P 87412-81-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 53645-78-6 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 1,4-diphenyl- (CA INDEX NAME)



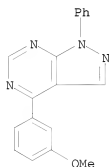
RN 87412-72-4 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(3-methylphenyl)-1-phenyl- (CA INDEX NAME)



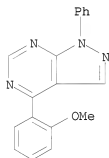
RN 87412-73-5 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(3-methylphenyl)-1-phenyl- (CA INDEX NAME)



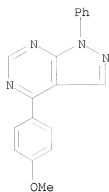
RN 87412-74-6 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(3-methoxyphenyl)-1-phenyl- (CA INDEX NAME)



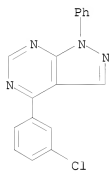
RN 87412-75-7 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(2-methoxyphenyl)-1-phenyl- (CA INDEX NAME)



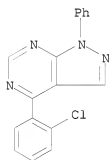
RN 87412-76-8 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(4-methoxyphenyl)-1-phenyl- (CA INDEX NAME)



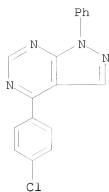
RN 87412-77-9 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(3-chlorophenyl)-1-phenyl- (CA INDEX NAME)



RN 87412-78-0 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(2-chlorophenyl)-1-phenyl- (CA INDEX NAME)

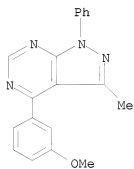


RN 87412-79-1 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(4-chlorophenyl)-1-phenyl- (CA INDEX NAME)



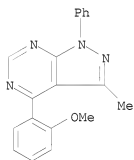
RN 87412-80-4 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(3-methoxyphenyl)-3-methyl-1-phenyl- (CA  
INDEX NAME)

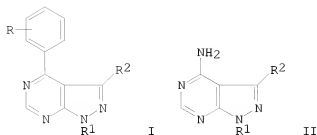


RN 87412-81-5 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(2-methoxyphenyl)-3-methyl-1-phenyl- (CA  
INDEX NAME)



GI



AB 4-Arylpyrazolo[3,4-d]pyrimidines I were prepared to evaluate their biol. activity. Attempts to prepare I from 4-aminopyrazolo[3,4-d]pyrimidines II via classical Comberg-Bachmann-Hey aryl coupling conditions failed. Conversion of II into I was accomplished by diazotization, using alkyl nitrites with an acid catalyst in aromatic solvents. Isomer distribution of I was that predicted for a radical intermediate (ortho > meta .simeq. para); isomer structures were assigned by <sup>1</sup>H NMR anal. Unusual fragmentation products were isolated during the course of investigations, which probably arose from collapse of intermediate pyrazolo[3,4-d]pyrimidin-4-yl radicals. Compds. prepared included I (R, R1, R2 = Me, Me, Me; Cl, Me, Me; MeO, Me, H).

ACCESSION NUMBER: 1982:472700 CAPLUS

DOCUMENT NUMBER: 97:72700

ORIGINAL REFERENCE NO.: 97:12181a,12184a

TITLE: Pyrazolo[3,4-d]pyrimidine ribonucleosides as anticoccidials. 2. Synthesis and activity of some nucleosides of 4-(alkylamino)-1H-pyrazolo[3,4-d]pyrimidines

AUTHOR(S): Rideout, Janet L.; Krenitsky, Thomas A.; Koszalka, George W.; Cohn, Naomi K.; Chao, Esther Y.; Elion, Gertrude B.; Latter, Victoria S.; Williams, Raymond B.  
CORPORATE SOURCE: Wellcome Res. Lab., Burroughs Wellcome Co., Research Triangle Park, NC, 27709, USA

SOURCE: Journal of Medicinal Chemistry (1982), 25(9), 1040-4  
CODEN: JMCMAR; ISSN: 0022-2623

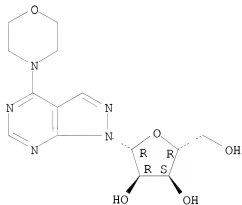
DOCUMENT TYPE: Journal  
LANGUAGE: English

IT 82436-65-5P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and anticoccidial activity of)

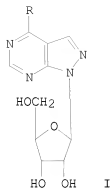
RN 82436-65-5 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(4-morpholinyl)-1-β-D-ribofuranosyl-  
(CA INDEX NAME)

Absolute stereochemistry.



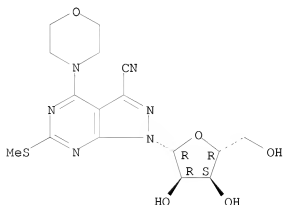
GI



AB A series of 4-(alkylamino)-1-β-D-ribofuranosyl-1H-pyrazolo[3,4-d]pyrimidines was synthesized by enzymic and chemical methods. On the basis of the previous finding that 4-(alkylthio)-1-β-D-ribofuranosyl-1H-pyrazolo[3,4-d]pyrimidines were effective anticoccidial agents, this series was examined for efficacy against *Eimeria tenella* in chicks. The most active anticoccidial agent in the study was I (R = cyclopentylamino), which cleared chicks of the parasite at 200 ppm in the diet. Some members of this series were toxic to embryonic chick liver cells, mouse cells, and human cells in vitro. I (R = Et<sub>2</sub>N), which was not toxic in vitro, was toxic to chicks.

L14 ANSWER 58 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1982:7014 CAPLUS  
 DOCUMENT NUMBER: 96:7014  
 ORIGINAL REFERENCE NO.: 96:1283a,1286a  
 TITLE: The nucleosides of substituted pyrazolo(3,4-d)pyrimidines  
 AUTHOR(S): Korbukh, I. A.; Bulychev, Yu. N.; Yakunina, N. G.; Preobrazhenskaya, M. N.  
 CORPORATE SOURCE: All-Union Cancer Res. Cent., Moscow, 115478, USSR  
 SOURCE: Nucleic Acids Symposium Series (1981), 9, 73-5  
 CODEN: NACSD8; ISSN: 0261-3166  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 IT 78724-03-5P 78724-04-6P 78724-05-7P  
 80117-84-6P 80117-85-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 78724-03-5 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine-3-carbonitrile, 6-(methylthio)-4-(4-morpholinyl)-1-β-D-ribofuranosyl- (CA INDEX NAME)

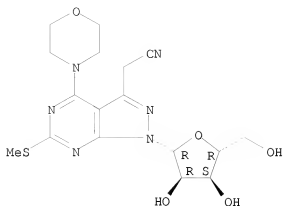
Absolute stereochemistry.



RN 78724-04-6 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine-3-acetonitrile, 6-(methylthio)-4-(4-morpholinyl)-1-β-D-ribofuranosyl- (CA INDEX NAME)

Absolute stereochemistry.

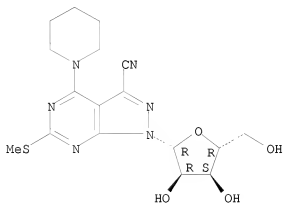




RN 78724-05-7 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine-3-carbonitrile, 6-(methylthio)-4-(1-piperidinyl)-1-β-D-ribofuranosyl- (CA INDEX NAME)

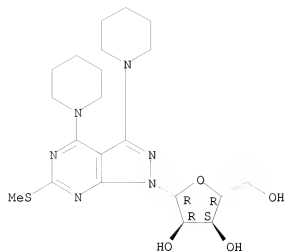
Absolute stereochemistry.



RN 80117-84-6 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-(methylthio)-3,4-di-1-piperidinyl-1-β-D-ribofuranosyl- (CA INDEX NAME)

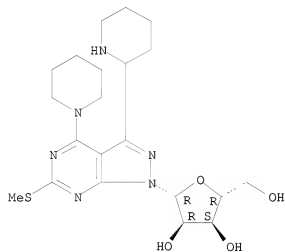
Absolute stereochemistry.



RN 80117-85-7 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-(methylthio)-4-(1-piperidinyl)-3-(2-piperidinyl)-1-β-D-ribofuranosyl- (CA INDEX NAME)

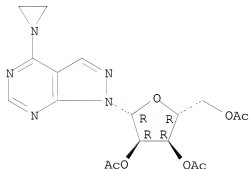
Absolute stereochemistry.



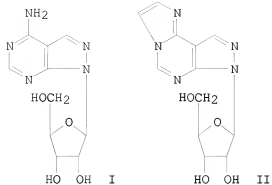
AB The 1-β-D-ribosides of 4-, 3,4-, 4,6- and 3,4,6-substituted pyrazolo[3,4-d]pyrimidines were prepared by regioselective glycosylation and subsequent transformations.

L14 ANSWER 59 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1981:620260 CAPLUS  
 DOCUMENT NUMBER: 95:220260  
 ORIGINAL REFERENCE NO.: 95:36765a,36768a  
 TITLE: Synthesis of certain fluorescent tricyclic nucleosides  
 derived from pyrazolo[3,4-d]pyrimidine nucleosides  
 AUTHOR(S): Bhat, Ganapati A.; Townsend, Leroy B.  
 CORPORATE SOURCE: Dep. Med. Chem., Univ. Michigan, Ann Arbor, MI, 48109,  
 USA  
 SOURCE: Journal of the Chemical Society, Perkin Transactions  
 1: Organic and Bio-Organic Chemistry (1972-1999)  
 (1981), (9), 2387-93  
 CODEN: JCPRB4; ISSN: 0300-922X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 IT 79974-30-4P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and reaction of, with sodium iodide, dihydroimidazole  
 derivative  
 by)  
 RN 79974-30-4 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(1-aziridinyl)-1-(2,3,5-tri-O-acetyl-  
 $\beta$ -D-ribofuranosyl)- (CA INDEX NAME)

Absolute stereochemistry.



GI



AB The preparation is described of tricyclic nucleosides with a dihydroimidazole, imidazole, triazole, or tetrazole ring fused to the pyrazolopyrimidine ring system in an angular position. E.g., cyclocondensation reaction of the nucleoside I with ClCH<sub>2</sub>CHO (H<sub>2</sub>O, NaOAc, pH 4.5, 80°, 3 h) gave the imidazo derivative II (64%). The UV and fluorescence spectra of the tricyclic nucleosides are reported.

L14 ANSWER 60 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1981:580745 CAPLUS

DOCUMENT NUMBER: 95:180745

ORIGINAL REFERENCE NO.: 95:30015a,30018a

TITLE: Antiviral activity of substituted 6-methylmercaptopyrazolo(3,4-d)pyrimidines and their ribosides

AUTHOR(S): Bektemirov, T. A.; Chekunova, E. V.; Korbukh, I. A.; Bulychev, Yu. N.; Yakunina, N. G.; Preobrazhenskaya, M. N.

CORPORATE SOURCE: Res. Inst. Virus Prep., Moscow, 109088, USSR

SOURCE: Acta Virologica (English Edition) (1981), 25(5), 326-9

CODEN: AVIRA2; ISSN: 0001-723X

DOCUMENT TYPE: Journal

LANGUAGE: English

IT 78724-03-5 78724-05-7

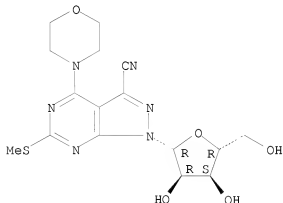
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(antiviral activity of)

RN 78724-03-5 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine-3-carbonitrile, 6-(methylthio)-4-(4-morpholinyl)-1-β-D-ribofuranosyl- (CA INDEX NAME)

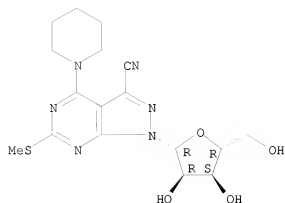
Absolute stereochemistry.



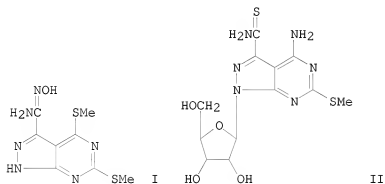
RN 78724-05-7 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine-3-carbonitrile, 6-(methylthio)-4-(1-piperidinyl)-1-β-D-ribofuranosyl- (CA INDEX NAME)

Absolute stereochemistry.



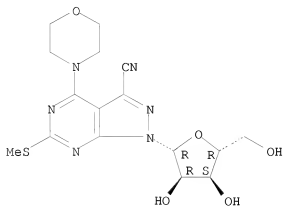
GI



AB Many pyrazolopyrimidine derivs. had antiviral activities, with I [74516-71-5] and II [74516-78-2] being the only compds. effective at concns. <250 µg/mL. The antiviral effects were screened against both herpes simplex type 1 and vaccinia virus in chick embryo cells, and the herpes virus was generally inhibited to the greater extent. All compds. that significantly inhibited viral replication contained a methylmercapto group, and most nucleosides were more active than the corresponding heterocyclic bases.

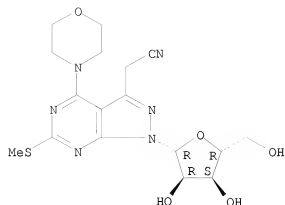
L14 ANSWER 61 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1981:498198 CAPLUS  
 DOCUMENT NUMBER: 95:98198  
 ORIGINAL REFERENCE NO.: 95:16523a,16526a  
 TITLE: Synthesis of derivatives of pyrazolo[3,4-d]pyrimidin-3-ylacetic acid and their nucleosides  
 AUTHOR(S): Bulychev, Yu. N.; Korbukh, I. A.; Preobrazhenskaya, M. N.  
 CORPORATE SOURCE: Onkol. Nauchn. Tsentr, Moscow, 115478, USSR  
 SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1981), (4), 536-45  
 CODEN: KGSSAQ; ISSN: 0453-8234  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 IT 78724-03-5P 78724-04-6P 78724-05-7P  
 78739-23-8P 78739-24-9P  
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)  
 RN 78724-03-5 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine-3-carbonitrile, 6-(methylthio)-4-(4-morpholinyl)-1-β-D-ribofuranosyl- (CA INDEX NAME)

Absolute stereochemistry.



RN 78724-04-6 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine-3-acetonitrile, 6-(methylthio)-4-(4-morpholinyl)-1-β-D-ribofuranosyl- (CA INDEX NAME)

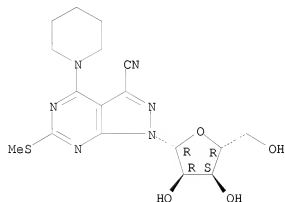
Absolute stereochemistry.



RN 78724-05-7 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine-3-carbonitrile, 6-(methylthio)-4-(1-piperidinyl)-1-β-D-ribofuranosyl- (CA INDEX NAME)

Absolute stereochemistry.

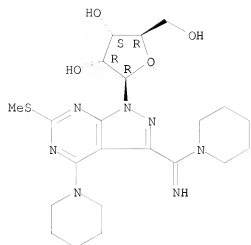


RN 78739-23-8 CAPLUS

CN Piperidine, 1-[imino[6-(methylthio)-4-(1-piperidinyl)-1-β-D-ribofuranosyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

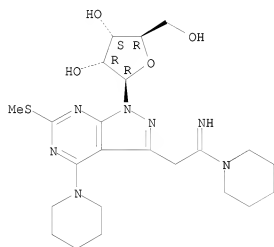




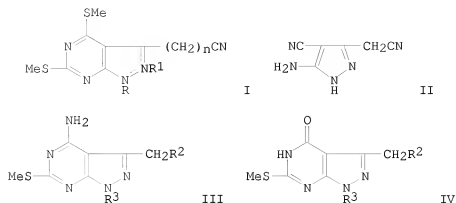
RN 78739-24-9 CAPLUS

CN Piperidine, 1-[1-imino-2-[6-(methylthio)-4-(1-piperidinyl)-1-β-D-ribofuranosyl-1H-pyrazolo[3,4-d]pyrimidin-3-yl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



GI



AB Pyrazolopyrimidine I ( $R = R_1 = H$ ,  $n = 1$ ), prepared in 87% yield from II by cyclocondensation with  $CS_2$ , hydrolysis, and methylation, were ribosylated by 1,2,3,5-tetra-O-acetyl- $\beta$ -D-ribofuranose to give I ( $R = 2,3,5$ -tri-O-acetyl- $\alpha$ , $\beta$ -D-ribofuranosyl,  $R_1 = H$ ,  $n = 1$ ;  $R = H$ ,  $R_1 = 2,3,5$ -tri-O-acetyl- $\beta$ -D-ribofuranosyl,  $n = 1$ ). Addnl. obtained were 54 and 40% III ( $R_2 = CO_2NH_4$ , CN,  $R_3 = \beta$ -D-ribofuranosyl) and 20 and 53% IV ( $R_2 = CN$ ,  $CONH_2$ ,  $R_3 = \beta$ -D-ribofuranosyl). Treatment of the 6-methylthio derivs. with morpholine and piperidine gave the corresponding amino derivs.

L14 ANSWER 62 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1979:54896 CAPLUS

DOCUMENT NUMBER: 90:54896

ORIGINAL REFERENCE NO.: 90:8781a,8784a

TITLE: Studies on pyrazolo[3,4-d]pyrimidine derivatives.  
XII. On 1-phenyl-1H-pyrazolo[3,4-d]pyrimidine-4-  
carboxylic acid

AUTHOR(S): Suzuki, Shinichi

CORPORATE SOURCE: Basic Res. Lab., Lion Dentifrice Co., Ltd., Odawara,  
Japan

SOURCE: Yakugaku Zasshi (1978), 98(9), 1274-8

CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

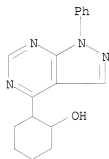
OTHER SOURCE(S): CASREACT 90:54896

IT 69001-66-7P

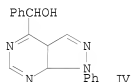
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 69001-66-7 CAPLUS

CN Cyclohexanol, 2-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)- (CA INDEX  
NAME)



GI



AB 1-Phenyl-1H-pyrazolo[3,4-d]pyrimidine-4-carboxylic acid (I) forms esters (II) with alcs., in the presence of an acid. II reacts with hydroxylamine, hydrazine, and amines to form hydroxamic acid, hydrazide, and amides, resp. I also forms a labile acid chloride (III) with thionyl chloride, and III reacts with alcs., amines, and thioalcs. to form esters, amides, and thioesters, resp. I easily undergoes decarboxylation to form 1-phenyl-1H-pyrazolo[3,4-d]pyrimidine. I undergoes the Hammick reaction, and decarboxylation by heating in the presence of a carbonyl compound affords a carbinol derivative (e.g. IV) a ketone formed by oxidation of the carbinol.



L14 ANSWER 63 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1978:615358 CAPLUS

DOCUMENT NUMBER: 89:215358

ORIGINAL REFERENCE NO.: 89:33465a,33468a

TITLE: Studies on pyrazolo[3,4-d]pyrimidine derivatives. XI.

AUTHOR(S): 1-Phenyl-1H-pyrazolo[3,4-d]pyrimidine-4-carbonitrile

CORPORATE SOURCE: Hayashi, Eisaku; Higashino, Takeo; Suzuki, Shinichi

SOURCE: Shizuoka Coll. Pharm., Shizuoka, Japan

Yakugaku Zasshi (1978), 98(7), 891-7

CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

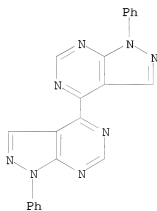
OTHER SOURCE(S): CASREACT 89:215358

IT 59563-52-9P 62141-19-9P 62141-20-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

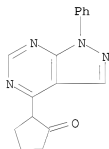
RN 59563-52-9 CAPLUS

CN 4,4'-Bi-1H-pyrazolo[3,4-d]pyrimidine, 1,1'-diphenyl- (CA INDEX NAME)



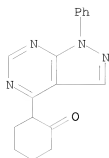
RN 62141-19-9 CAPLUS

CN Cyclopentanone, 2-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)- (CA INDEX NAME)

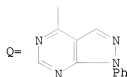


RN 62141-20-2 CAPLUS

CN Cyclohexanone, 2-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)- (CA INDEX NAME)



GI



AB Cyanation of QCl or QSO<sub>2</sub>C<sub>6</sub>H<sub>4</sub>Me-p in Me<sub>2</sub>SO gave the title compound QCN (I). Nucleophilic substitution of the CN group in I took place with NaOH, NaOMe, amines, hydrazines and carbanions (active methylene compds. or ketones in the presence of NaNH<sub>2</sub>). Addition to CN in I occurred in acid hydrolysis, reaction with H<sub>2</sub>O<sub>2</sub>-alkali, NH<sub>2</sub>OH, and H<sub>2</sub>S giving acid, amide, amidoxime and thiocarboxamide, resp. Reduction of I by Raney Ni in HCO<sub>2</sub>H gave QCH<sub>2</sub>NH<sub>2</sub> and QH.

ACCESSION NUMBER: 1978:170081 CAPLUS

DOCUMENT NUMBER: 88:170081

ORIGINAL REFERENCE NO.: 88:26810h,26811a

TITLE: Studies on pyrazolo[3,4-d]pyrimidine derivatives. IX.  
4-(p-Tolylsulfonyl)-1-phenyl-1H-pyrazolo[3,4-d]pyrimidine

AUTHOR(S): Hayashi, Eisaku; Higashino, Takeo; Suzuki, Shinichi

CORPORATE SOURCE: Shizuoka Coll. Pharm., Shizuoka, Japan

SOURCE: Yakugaku Zasshi (1978), 98(1), 89-94

CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

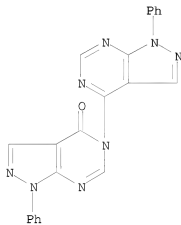
OTHER SOURCE(S): CASREACT 88:170081

IT 66370-43-2P

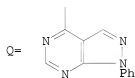
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 66370-43-2 CAPLUS

CN [4,5'-(4'H)-Bi-1H-pyrazolo[3,4-d]pyrimidin]-4'-one, 1,1'-diphenyl- (CA  
INDEX NAME)



GI



AB 4-(P-tolylsulfonyl)-1-phenyl-1H-pyrazolo[3,4-d]pyrimidine, QS02C6H4Me-4, was hydrolyzed by dilute HCl to give 1,5-dihydro-1-phenyl-4H-pyrazolo[3,4-d]pyrimidin-4-one (I), and the p-tolylsulfonyl group underwent nucleophilic substitution with hydroxide, methoxides, hydrazine, BuNH2, aniline, and cyanides. Application of active methylene compds., nitriles, or ketones in the presence of NaNH2 resulted in substitution with a carbanion. When a ketone was used as the carbanion source, reaction differed with reaction conditions. E.g., the use of acetone resulted in

the formation of 1-Q-substituted-2-propanone or 1,1-bis-Q-substituted-2-propanone. When 2-butanone was used, the product was either 3-Q-substituted-2-butanone or 1,1-bis-Q-substituted-2-butanone. In these cases, I was formed at the same time and its process of formation is discussed. In some cases 5-Q-substituted-1,5-dihydro-1-phenyl-4H-pyrazolo[3,4-d]pyrimidin-4-one was formed as a by-product.



L14 ANSWER 65 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1978:44881 CAPLUS

DOCUMENT NUMBER: 88:44881

ORIGINAL REFERENCE NO.: 88:6997a,7000a

TITLE: Antitumor activity of eighty-four synthesized N-heteroaromatic compounds

AUTHOR(S): Hayashi, Eisaku; Higashino, Takeo; Iijima, Chihoko; Oishi, Etsuo; Makino, Hirokazu; Irie, Toshio; Yamamoto, Fusako; Yokoyama, Yoko; Iwai, Yoshihisa; et al.

CORPORATE SOURCE: Shizuoka Coll. Pharm., Shizuoka, Japan

SOURCE: Yakugaku Zasshi (1977), 97(9), 1022-33

CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

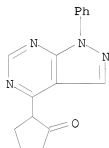
OTHER SOURCE(S): CASREACT 88:44881

IT 62141-19-9P 62141-20-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation and antitumor activity of)

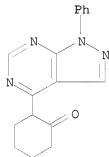
RN 62141-19-9 CAPLUS

CN Cyclopentanone, 2-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)- (CA INDEX NAME)

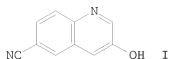


RN 62141-20-2 CAPLUS

CN Cyclohexanone, 2-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)- (CA INDEX NAME)

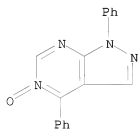


GI

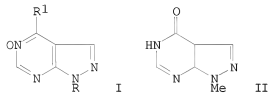


AB Eighty-four compds. (mainly N-heteroarom. compds.) were synthesized and their antitumor activity was examined. Four quinoline derivs. had some antitumor effect on the solid type of Ehrlich carcinoma. These compds. were, 3-hydroxy-6-quinolinecarbonitrile (I) [63124-12-9], 6-bromoquinaldic acid 1-oxide [65147-79-7], 8-(hydroxyimino)-5,6,7,8-tetrahydroquinoline [58509-59-4] and 1-(hydroxyimino)-1,2,3,4-tetrahydroacridine [34043-68-0]. No other derivs. were found effective.

L14 ANSWER 66 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1978:21567 CAPLUS  
 DOCUMENT NUMBER: 88:21567  
 ORIGINAL REFERENCE NO.: 88:3465a,3468a  
 TITLE: Studies on pyrazolo[3,4-d]pyrimidine derivatives.  
 VII. Mass spectra of pyrazolo[3,4-d]pyrimidine  
 5-oxides  
 AUTHOR(S): Uchida, Mitsuo; Higashino, Takeo; Hayashi, Eisaku  
 CORPORATE SOURCE: Shizuoka Coll. Pharm., Shizuoka, Japan  
 SOURCE: Shitsuryo Bunseki (1977), 25(2), 161-8  
 CODEN: SHIBAK; ISSN: 0542-8645  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 IT 62564-80-1  
 RL: PRP (Properties)  
 (mass spectra of)  
 RN 62564-80-1 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 1,4-diphenyl-, 5-oxide (CA INDEX NAME)



GI



AB Mass spectra of I (R = Me, R1 = H; R = Ph, R1 = H; R = Ph, R1 = Me2CH; R = R1 = Ph; R = Ph, R1 = PhCO) and II were examined. The possible principle fragmentation of I and II is summarized by four dissociation paths. The pressure dependency is widely observed for many of the fragment ions.

L14 ANSWER 67 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1977:171372 CAPLUS

DOCUMENT NUMBER: 86:171372

ORIGINAL REFERENCE NO.: 86:26920h,26921a

TITLE: Studies on pyrazolo[3,4-d]pyrimidine derivatives. IV.  
On 1-methyl- and 1-phenyl-1H-pyrazolo[3,4-d]pyrimidine  
5-oxide

AUTHOR(S): Higashino, Takeo; Iwai, Yoshihisa; Hayashi, Eisaku

CORPORATE SOURCE: Shizuoka Coll. Pharm., Shizuoka, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1976), 24(12),  
3120-34

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 86:171372

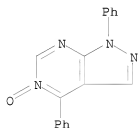
IT 62564-80-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(preparation and deoxygenation of)

RN 62564-80-1 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1,4-diphenyl-, 5-oxide (CA INDEX NAME)

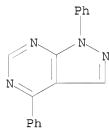


IT 53645-78-6P

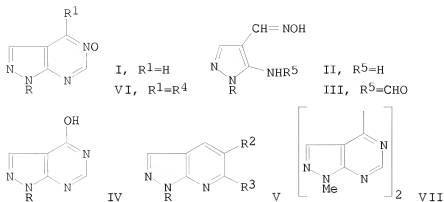
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 53645-78-6 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1,4-diphenyl- (CA INDEX NAME)

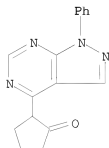


GI

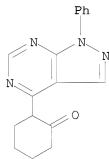


AB The title compds. I (R = Me, Ph), prepared by cyclization of the pyrazoles II with HC(OEt)<sub>3</sub>, reacted with 1 N NaOH, Ac<sub>2</sub>O, R<sub>2</sub>CH<sub>2</sub>R<sub>3</sub> (R<sub>2</sub> = R<sub>3</sub> = CN, CO<sub>2</sub>Et, COMe; R<sub>2</sub> = MeCO, R<sub>3</sub> = CO<sub>2</sub>Et) and R<sub>4</sub>MgX (R<sub>4</sub> = Me<sub>2</sub>CH, Ph, PhCH<sub>2</sub>, Me, Et) to give III-VI. Thermal decomposition of II (R = Me) at 170° gave the bis(pyrazolopyrimidine) VII.

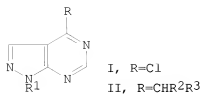
ACCESSION NUMBER: 1977:121280 CAPLUS  
 DOCUMENT NUMBER: 86:121280  
 ORIGINAL REFERENCE NO.: 86:19155a,19158a  
 TITLE: Studies on pyrazolo[3,4-d]pyrimidine derivatives.  
 III. The reaction of 1-methyl- and  
 1-phenyl-4-chloro-1H-pyrazolo[3,4-d]pyrimidine with  
 carbanion  
 AUTHOR(S): Higashino, Takeo; Iwai, Yoshihisa; Hayashi, Eisaku  
 CORPORATE SOURCE: Shizuoka Coll. Pharm., Shizuoka, Japan  
 SOURCE: Yakugaku Zasshi (1976), 96(11), 1352-6  
 CODEN: YKKZAJ; ISSN: 0031-6903  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Japanese  
 IT 62141-19-9P 62141-20-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 62141-19-9 CAPLUS  
 CN Cyclohexanone, 2-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)- (CA INDEX  
 NAME)



RN 62141-20-2 CAPLUS  
 CN Cyclohexanone, 2-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)- (CA INDEX  
 NAME)



GI



AB The pyrazolopyrimidines I (R<sub>1</sub> = Me, Ph) reacted with R<sub>2</sub>CH<sub>2</sub>R<sub>3</sub> [R<sub>2</sub>, R<sub>3</sub> = H, CN, CO<sub>2</sub>Et, Ph, COMe, CPh or R<sub>2</sub>R<sub>3</sub> = (CH<sub>2</sub>)<sub>4</sub>CO] in benzene containing NaNH<sub>2</sub> to give II in 3.7-78.9% yields.

ACCESSION NUMBER: 1977:105189 CAPLUS

DOCUMENT NUMBER: 86:105189

ORIGINAL REFERENCE NO.: 86:16589a,16592a

TITLE: Studies on pyrazolo[3,4-d]pyrimidine derivatives. VI. Mass spectra of 1-methyl (or phenyl)-1H-pyrazolo[3,4-d]pyrimidines

AUTHOR(S): Higashino, Takeo; Uchida, Mitsuo; Hayashi, Eisaku

CORPORATE SOURCE: Shizuoka Coll. Pharm., Shizuoka, Japan

SOURCE: Shitsuryo Bunseki (1976), 24(2), 189-98

CODEN: SHIBAK; ISSN: 0542-8645

DOCUMENT TYPE: Journal

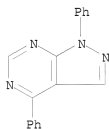
LANGUAGE: English

IT 53645-78-6

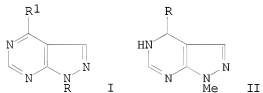
RL: PRP (Properties)  
(mass spectrum of)

RN 53645-78-6 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1,4-diphenyl- (CA INDEX NAME)



GI



AB Mass spectra of 1H-pyrazolo[3,4-d]pyrimidines I (R = Me or Ph; R1 = H, Me, Et, CHMe2, CH2Ph, Ph) and II (R = Me, Et, CHMe2, CH2Ph, Ph) were examined. The main fragmentation of I proceeds by 2 dissociation paths. One is the formation of a pyrazolo[3,4-d]pyrimidinium cation, or the mol. ion caused by the elimination of the 4-substituent, with fragmentation of the condensed pyrimidine ring of the resulting ion, leading to a pyrazolyne radical ion by the loss of HCN or cyano radical in successive steps. Another is the formation of a cyclic ion or diazatropyrium type ion caused by the migration of the 4-substituent with the loss of H radical. The main fragmentation of II is the elimination of the 4-substituent to form a pyrazolo[3,4-d]pyrimidinium ion.



ACCESSION NUMBER: 1976:421290 CAPLUS

DOCUMENT NUMBER: 85:21290

ORIGINAL REFERENCE NO.: 85:3481a,3484a

TITLE: Studies on the reaction of  $\pi$ -deficient heterocycles

with aromatic aldehydes in the presence of cyanide ion

AUTHOR(S): Higashino, Takeo; Goi, Masami; Hayashi, Eisaku

CORPORATE SOURCE: Shizuoka Coll. Pharm., Shizuoka, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1976), 24(2), 238-52

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

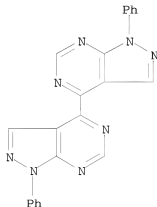
OTHER SOURCE(S): CASREACT 85:21290

IT 59563-52-9P

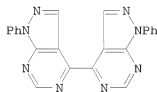
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 59563-52-9 CAPLUS

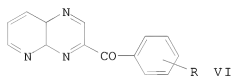
CN 4,4'-Bi-1H-pyrazolo[3,4-d]pyrimidine, 1,1'-diphenyl- (CA INDEX NAME)



GI



IV



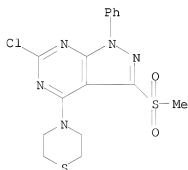
VI

AB Dimerization of  $\pi$ -deficient heterocycles was catalyzed by cyanide ion in Me2SO. Thus, reaction of quinoxaline, 1-phenyl-1H-pyrazolo[3,4-d]pyrimidine(I), 1-methyl-1H-pyrazolo[3,4-d]pyrimidine (II), and pyrido[2,3-b]pyrazine (III) with cyanide ion gave 2,2'-bi-quinoxaline, 4,4'-bis[1-phenyl-1H-pyrazolo[3,4-d]pyrimidine] (IV), 4,4'-bis[1-methyl-1H-pyrazolo[3,4-d]pyrimidine], and 2,2'-bispyrido[2,3-b]pyrazine, resp., although the yields of these dimers were very poor.  $\pi$ -Deficient heterocycles with RC6H4CHO (V, R = o-, m-, p-MeO, Cl, Me, etc.) in the presence of cyanide ion in Me2SO underwent a cross benzoin condensation

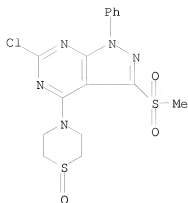
reaction. Thus, 4-isoquinolinecarbonitrile reacted with V to give  $\alpha$ -aryl-4-cyano-1-isoquinolinemethanol and aryl 4-cyano-1-isoquinolyl ketone together with 1,1'-biisoquinoline-4,4'-dicarbonitrile. Similarly, quinoxaline and V gave  $\alpha$ -aryl-2-quinoxalinemethanol and aryl 2-quinoxalinyl ketone, I and V gave  $\alpha$ -aryl-1-phenyl-1H-pyrazolo[3,4-d]pyrimidine-4-methanol and aryl 1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl ketone, II and V produced  $\alpha$ -aryl-1-methyl-1H-pyrazolo[3,4-d]pyrimidine-4-methanol and aryl 1-methyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl ketone, and III and V formed aryl 2-pyrido[2,3-b]pyrazinyl ketone VI.

ACCESSION NUMBER: 1976:135709 CAPLUS  
 DOCUMENT NUMBER: 84:135709  
 ORIGINAL REFERENCE NO.: 84:22063a,22066a  
 TITLE: Pyrazolo[3,4-d]pyrimidines  
 INVENTOR(S): Mueller, Erich; Nickl, Josef; Roch, Josef; Narr, Berthold  
 PATENT ASSIGNEE(S): Thomae, Dr. Karl, G.m.b.H., Fed. Rep. Ger.  
 SOURCE: Ger. Offen., 33 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2430454	A1	19760115	DE 1974-2430454	19740625
PRIORITY APPLN. INFO.:			DE 1974-2430454	A 19740625
IT 58732-65-3	58732-67-5	58732-68-6		
58732-70-0	58732-77-7	58732-78-8		
58732-80-2	58732-83-5	58732-85-7		
58732-88-0	58732-90-4	58732-95-9		
58732-97-1				
RL: RCT (Reactant); RACT (Reactant or reagent) (amination of)				
RN 58732-65-3	CAPLUS			
CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-chloro-3-(methylsulfonyl)-1-phenyl-4-(4-thiomorpholinyl)-	(CA INDEX NAME)			

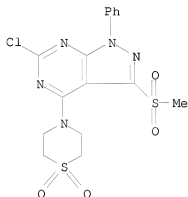


RN 58732-67-5 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-chloro-3-(methylsulfonyl)-4-(1-oxido-4-thiomorpholinyl)-1-phenyl- (CA INDEX NAME)



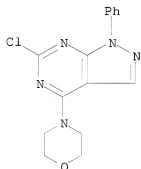
RN 58732-68-6 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-chloro-4-(1,1-dioxido-4-thiomorpholinyl)-3-(methylsulfonyl)-1-phenyl- (CA INDEX NAME)



RN 58732-70-0 CAPLUS

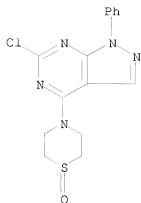
CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-chloro-4-(4-morpholinyl)-1-phenyl- (CA INDEX NAME)



RN 58732-77-7 CAPLUS

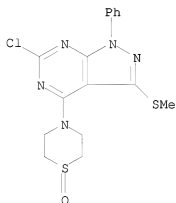
CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-chloro-4-(1-oxido-4-thiomorpholinyl)-1-phenyl-

phenyl- (CA INDEX NAME)



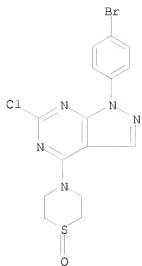
RN 58732-78-8 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-chloro-3-(methylthio)-4-(1-oxido-4-thiomorpholinyl)-1-phenyl- (CA INDEX NAME)



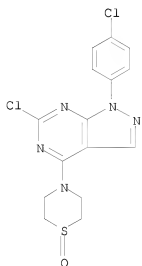
RN 58732-80-2 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-(4-bromophenyl)-6-chloro-4-(1-oxido-4-thiomorpholinyl)- (CA INDEX NAME)



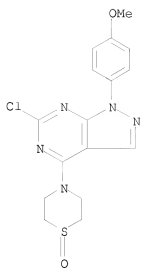
RN 58732-83-5 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-chloro-1-(4-chlorophenyl)-4-(1-oxido-4-thiomorpholinyl)- (CA INDEX NAME)



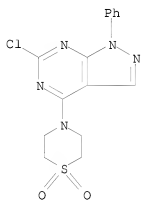
RN 58732-85-7 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-chloro-1-(4-methoxyphenyl)-4-(1-oxido-4-thiomorpholinyl)- (CA INDEX NAME)



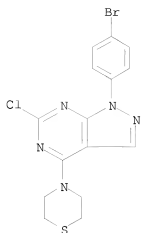
RN 58732-88-0 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-chloro-4-(1,1-dioxido-4-thiomorpholinyl)-1-phenyl- (CA INDEX NAME)



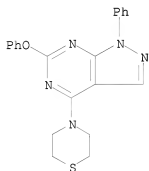
RN 58732-90-4 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-(4-bromophenyl)-6-chloro-4-(4-thiomorpholinyl)- (CA INDEX NAME)



RN 58732-95-9 CAPLUS

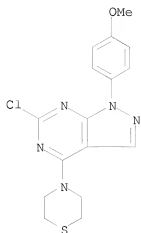
CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-phenoxy-1-phenyl-4-(4-thiomorpholinyl)-  
(CA INDEX NAME)



RN 58732-97-1 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-chloro-1-(4-methoxyphenyl)-4-(4-thiomorpholinyl)- (CA INDEX NAME)





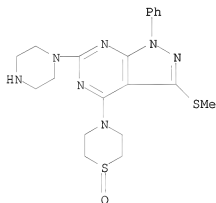
IT 58732-82-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and oxidation of)

RN 58732-82-4 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 3-(methylthio)-4-(1-oxido-4-thiomorpholinyl)-1-phenyl-6-(1-piperazinyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

IT 58732-66-4P 58732-69-7P 58732-71-1P

58732-72-2P 58732-73-3P 58732-74-4P

58732-75-5P 58732-76-6P 58732-79-9P

58732-81-3P 58732-84-6P 58732-86-8P

58732-87-9P 58732-89-1P 58732-91-5P

58732-93-7P 58732-94-8P 58732-96-0P

58732-98-2P 58733-08-7P 58933-15-6P

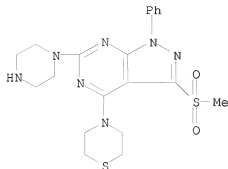
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 58732-66-4 CAPLUS

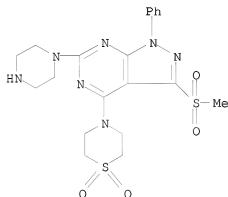
CN 1H-Pyrazolo[3,4-d]pyrimidine, 3-(methylsulfonyl)-1-phenyl-6-(1-

piperazinyl)-4-(4-thiomorpholinyl)- (CA INDEX NAME)



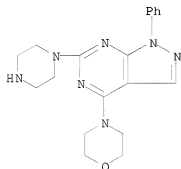
RN 58732-69-7 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(1,1-dioxido-4-thiomorpholinyl)-3-(methylsulfonyl)-1-phenyl-6-(1-piperazinyl)- (CA INDEX NAME)



RN 58732-71-1 CAPLUS

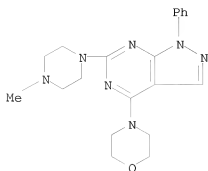
CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(4-morpholinyl)-1-phenyl-6-(1-piperazinyl)- (CA INDEX NAME)



RN 58732-72-2 CAPLUS

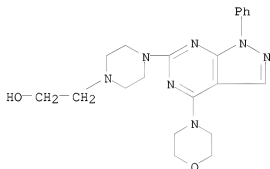
CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-(4-methyl-1-piperazinyl)-4-(4-morpholinyl)-

1-phenyl- (CA INDEX NAME)



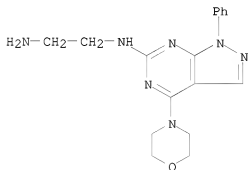
RN 58732-73-3 CAPLUS

CN 1-Piperazineethanol, 4-[4-(4-morpholinyl)-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]- (CA INDEX NAME)



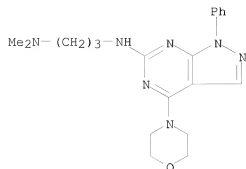
RN 58732-74-4 CAPLUS

CN 1,2-Ethanediamine, N-[4-(4-morpholinyl)-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]- (9CI) (CA INDEX NAME)



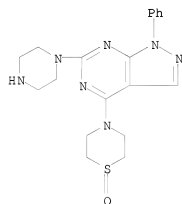
RN 58732-75-5 CAPLUS

CN 1,3-Propanediamine, N,N-dimethyl-N'-[4-(4-morpholinyl)-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]- (9CI) (CA INDEX NAME)



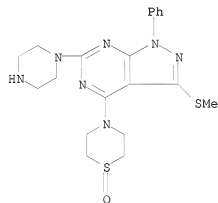
RN 58732-76-6 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(1-oxido-4-thiomorpholinyl)-1-phenyl-6-(1-piperazinyl)- (CA INDEX NAME)



RN 58732-79-9 CAPLUS

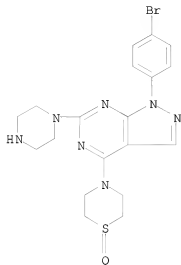
CN 1H-Pyrazolo[3,4-d]pyrimidine, 3-(methylthio)-4-(1-oxido-4-thiomorpholinyl)-1-phenyl-6-(1-piperazinyl)- (CA INDEX NAME)



RN 58732-81-3 CAPLUS

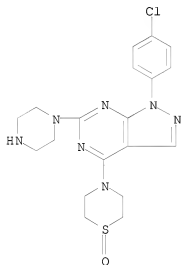
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-(4-bromophenyl)-4-(1-oxido-4-

thiomorpholinyl)-6-(1-piperazinyl)- (CA INDEX NAME)



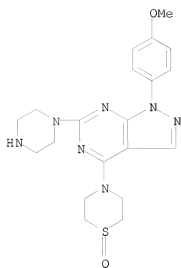
RN 58732-84-6 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-(4-chlorophenyl)-4-(1-oxido-4-thiomorpholinyl)-6-(1-piperazinyl)- (CA INDEX NAME)



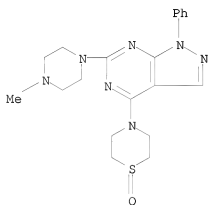
RN 58732-86-8 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-(4-methoxyphenyl)-4-(1-oxido-4-thiomorpholinyl)-6-(1-piperazinyl)- (CA INDEX NAME)



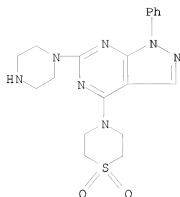
RN 58732-87-9 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-(4-methyl-1-piperazinyl)-4-(1-oxido-4-thiomorpholinyl)-1-phenyl- (CA INDEX NAME)



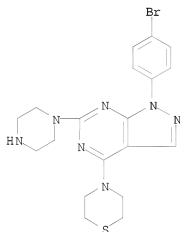
RN 58732-89-1 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(1,1-dioxido-4-thiomorpholinyl)-1-phenyl-6-(1-piperazinyl)- (CA INDEX NAME)



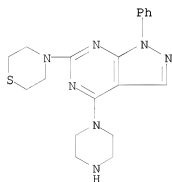
RN 58732-91-5 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-(4-bromophenyl)-6-(1-piperazinyl)-4-(4-thiomorpholinyl)- (CA INDEX NAME)



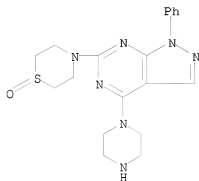
RN 58732-93-7 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-phenyl-4-(1-piperazinyl)-6-(4-thiomorpholinyl)- (CA INDEX NAME)



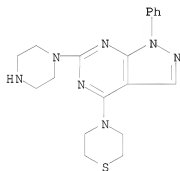
RN 58732-94-8 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-(1-oxido-4-thiomorpholinyl)-1-phenyl-4-(1-piperazinyl)- (CA INDEX NAME)



RN 58732-96-0 CAPLUS

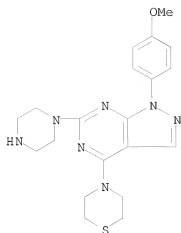
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-phenyl-6-(1-piperazinyl)-4-(4-thiomorpholinyl)- (CA INDEX NAME)



RN 58732-98-2 CAPLUS

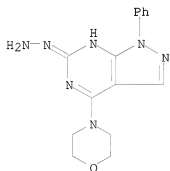
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-(4-methoxyphenyl)-6-(1-piperazinyl)-4-(4-thiomorpholinyl)- (CA INDEX NAME)





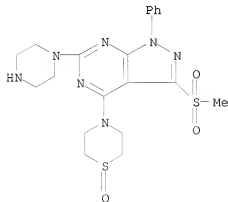
RN 58733-08-7 CAPLUS

CN 6H-Pyrazolo[3,4-d]pyrimidin-6-one, 1,5-dihydro-4-(4-morpholinyl)-1-phenyl-, hydrazone (9CI) (CA INDEX NAME)

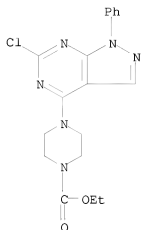


RN 58933-15-6 CAPLUS

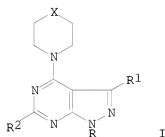
CN 1H-Pyrazolo[3,4-d]pyrimidine, 3-(methanesulfonyl)-4-(1-oxido-4-thiomorpholinyl)-1-phenyl-6-(1-piperazinyl)- (CA INDEX NAME)



IT 58732-92-6  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with thiomorpholine)  
 RN 58732-92-6 CAPLUS  
 CN 1-Piperazinecarboxylic acid, 4-(6-chloro-1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)-, ethyl ester (CA INDEX NAME)

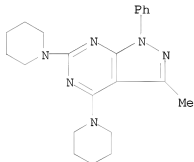


GI

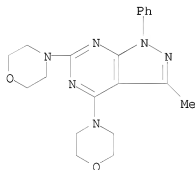


AB Pyrazolopyrimidines I (R = H, Ph, 4-BrC<sub>6</sub>H<sub>4</sub>, 4-ClC<sub>6</sub>H<sub>4</sub>, 4-MeOC<sub>6</sub>H<sub>4</sub>; R<sub>1</sub> = H, SO<sub>2</sub>Me, SMe, Me; R<sub>2</sub> = piperazino, substituted piperazino, NHCH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub>, NH(CH<sub>2</sub>)<sub>3</sub>NMe<sub>2</sub>, NHNH<sub>2</sub>; X = O, S, SO, SO<sub>2</sub>) (40 compds.) were prepared by aminating I (R<sub>2</sub> = Cl). I (R<sub>2</sub> = amino) are platelet aggregation inhibitors. Thus, I (R = R<sub>1</sub> = H, R<sub>2</sub> = N-methylpiperazino, X = S, SO; R = H, Me, R<sub>1</sub> = H, R<sub>2</sub> = piperazino, X = SO) had oral ED<sub>50</sub> in the Morris test of 5 + 10<sup>-6</sup> + 10<sup>-5</sup> mg/kg.

L14 ANSWER 72 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1976:17265 CAPLUS  
 DOCUMENT NUMBER: 84:17265  
 ORIGINAL REFERENCE NO.: 84:2859a,2862a  
 TITLE: Cycloacylation of enamines. IV. Synthesis of  
 1H-pyrazolo[3,4-d]pyrimidines  
 AUTHOR(S): Grohe, Klaus  
 CORPORATE SOURCE: Zent. Forsch., Bayer A.-G., Leverkusen, Fed. Rep. Ger.  
 SOURCE: Synthesis (1975), (10), 645-7  
 CODEN: SYNTBF; ISSN: 0039-7881  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German  
 OTHER SOURCE(S): CASREACT 84:17265  
 IT 57552-61-1P 57552-62-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 57552-61-1 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 3-methyl-1-phenyl-4,6-di-1-piperidinyl- (CA  
 INDEX NAME)



RN 57552-62-2 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 3-methyl-4,6-di-4-morpholinyl-1-phenyl- (CA  
 INDEX NAME)



GI For diagram(s), see printed CA Issue.  
 AB Cyclocondensation of aminopyrazoles I (R1 = Ph, CH2Ph, allyl; R2 = Me, Ph, allyl) with methanimines R3CC1:NCC12R4 (R3 = R4, = Cl, CC13) gave pyrazolopyrimidines II. R3 alone or R3 and R4 of II (R3 = R4 = Cl) were replaced by NH3, primary and secondary amines, and hydrazine to give

amino- [II, R3 = NHR5 (R5 = H, Me, Et, CHMe2), R4 = Cl] or  
 diaminopyrazolopyrimidines [II, R3 = NR5R6 (R5 = H, R6 = Et; R5R6 = (CH2)5,  
 (CH2)2O(CH2)2]; R4 = NR7R8 (R7 = H, R8 = Et, NH2; R7R8 = (CH2)5,  
 (CH2)2O(CH2)2]]. Hydrolysis of II (R1 = Ph, R2 = Me, R3 = R4 = Cl) gave  
 pyrazolopyrimidinedione III, also obtained from I and ClCONCO.

L14 ANSWER 73 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1975:409956 CAPLUS

DOCUMENT NUMBER: 83:9956

ORIGINAL REFERENCE NO.: 83:1661a,1664a

TITLE: Pyrimidines. XLIV. Synthesis of pyrazolo[3,4-d]pyrimidines

AUTHOR(S): Mikhaleva, M. A.; Il'chenko, L. N.; Mamaev, V. P.

CORPORATE SOURCE: Novosib. Inst. Org. Khim., Novosibirsk, USSR

SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1975), (1), 95-7

CODEN: KGSSAQ; ISSN: 0132-6244

DOCUMENT TYPE: Journal

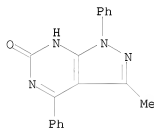
LANGUAGE: Russian

IT 55360-99-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 55360-99-1 CAPLUS

CN 6H-Pyrazolo[3,4-d]pyrimidin-6-one, 1,7-dihydro-3-methyl-1,4-diphenyl- (CA INDEX NAME)



GI For diagram(s), see printed CA Issue.

AB Boiling 1-phenyl-3-methyl-5-aminopyrazole with PhCH(NHCONH2)2 in AcOH 5 hr gave pyrazolopyrimidine (I), which was dehydrogenated by Br-AcOH to give 60% II. Boiling 1-phenyl-3-methyl-4-benzylidene-5-pyrazolone with urea 8 hr in alc. containing H2SO4 gave spiro derivative (III).

L14 ANSWER 74 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1974:520562 CAPLUS

DOCUMENT NUMBER: 81:120562

ORIGINAL REFERENCE NO.: 81:19063a,19066a

TITLE: Pyrazolo[3,4-d]pyrimidine derivatives. I. Reactions of 1-methyl- and 1-phenyl-1H-pyrazolo[3,4-d]pyrimidine with Grignard reagents

AUTHOR(S): Higashino, Takeo; Iwai, Yoshihisa; Hayashi, Eisaku

CORPORATE SOURCE: Shizuoka Coll. Pharm., Shizuoka, Japan

SOURCE: Yakugaku Zasshi (1974), 94(6), 666-71

CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal

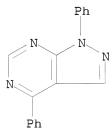
LANGUAGE: Japanese

IT 53645-78-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 53645-78-6 CAPLUS

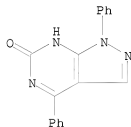
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1,4-diphenyl- (CA INDEX NAME)



GI For diagram(s), see printed CA Issue.

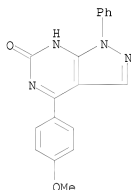
AB The pyrazolopyrimidines I (R = Me, Ph; R1 = H) were treated with Grignard reagents to give dihydropyrazolopyrimidines II (R = Me, Ph; R1 = Me, Et, Me2CH, PhCH2, Ph) which were oxidized with K2Fe(CN)6 to give I.

L14 ANSWER 75 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1974:413456 CAPLUS  
 DOCUMENT NUMBER: 81:13456  
 ORIGINAL REFERENCE NO.: 81:2166h,2167a  
 TITLE: Pyrimidines. XXXIX. Dehydrating action of  
 arylidenebisureas  
 AUTHOR(S): Mikhaleva, M. A.; Romanovskaya, S. A.; Belova, N. M.;  
 Sedova, V. F.; Mamaev, V. P.  
 CORPORATE SOURCE: Novosib. Inst. Org. Khim., Novosibirsk, USSR  
 SOURCE: Zhurnal Organicheskoi Khimii (1974), 10(4), 859-62  
 CODEN: ZORKAE; ISSN: 0514-7492  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 IT 35026-01-8P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 35026-01-8 CAPLUS  
 CN 6H-Pyrazolo[3,4-d]pyrimidin-6-one, 1,5-dihydro-1,4-diphenyl- (9CI) (CA  
 INDEX NAME)



GI For diagram(s), see printed CA Issue.  
 AB Dehydrogenation of pyrimidine I (R = R1 = Ph) by R2CH(NHCONH2)2 (II; R2 = Ph, p-MeOC6H4, p-Cl-C6H4) in BuOH 3 hr at 135° gave 34-80% pyrimidinone (III). Analogously I (R = Ph, R1 = p-MeOC6H4), dehydrogenated by II (R2 = Ph, p-MeOC6H4), yielded 62% of the corresponding III. Similar dehydrogenation of IV, V, and VI with II (R2 = Ph) gave 48% 1,2,5,6-tetrahydro derivative, 21% 3,4-dihydro derivative, and 55% 6,7-dihydro derivs., resp.

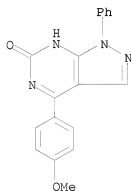
L14 ANSWER 76 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1974:150879 CAPLUS  
 DOCUMENT NUMBER: 80:150879  
 ORIGINAL REFERENCE NO.: 80:24329a,24332a  
 TITLE: Generation of the second harmonic of a neodymium laser  
 in derivatives of pyrimidines and fluorine-substituted  
 derivatives of benzene  
 AUTHOR(S): Davydov, B. L.; Zolin, V. F.; Koreneva, L. G.;  
 Samokhina, M. A.; Sedova, V. F.  
 CORPORATE SOURCE: USSR  
 SOURCE: Zhurnal Prikladnoi Spektroskopii (1974), 20(3), 516-18  
 CODEN: ZPSBAX; ISSN: 0514-7506  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 IT 35016-13-8  
 RL: PRP (Properties)  
 (second harmonic generation by, nonlinear susceptibility and charge  
 transfer effects on)  
 RN 35016-13-8 CAPLUS  
 CN 6H-Pyrazolo[3,4-d]pyrimidin-6-one, 1,5-dihydro-4-(4-methoxyphenyl)-1-  
 phenyl- (9CI) (CA INDEX NAME)



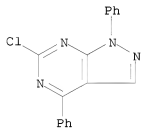
AB The relation between the nonlinear susceptibility, which is responsible  
 for 2nd harmonic generation, and intramol. charge transfer was studied for  
 pyrimidine derivs. and 20 halogen-substituted benzene derivs. All were  
 studied as powder (50-100  $\mu$ ), and their uv and visible absorption  
 spectra were recorded. Charge-transfer bands were found at 250-320 nm.  
 Many of the compds. did not give 2nd harmonic generation due to the  
 presence of an inversion center. The efficiency of 2nd harmonic  
 generation was connected with charge transfer occurring on excitation.  
 All studied F-containing compds. showed low efficiency for 2nd harmonic  
 generation.



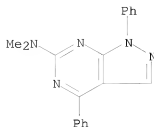
L14 ANSWER 77 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1972:25244 CAPLUS  
 DOCUMENT NUMBER: 76:25244  
 ORIGINAL REFERENCE NO.: 76:4103a,4106a  
 TITLE: Pyrimidines. XXIX. 4-Aryl-6-oxypyrazolo[3,4-d]pyrimidines  
 AUTHOR(S): Mamaev, V. P.; Mikhaleva, M. A.  
 CORPORATE SOURCE: Novosib. Inst. Org. Khim., Novosibirsk, USSR  
 SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1971), 7(4), 535-9  
 CODEN: KGSSAQ; ISSN: 0132-6244  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 IT 35016-13-8P 35016-14-9P 35016-17-2P  
 35016-20-7P 35026-01-8P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 35016-13-8 CAPLUS  
 CN 6H-Pyrazolo[3,4-d]pyrimidin-6-one, 1,5-dihydro-4-(4-methoxyphenyl)-1-phenyl- (9CI) (CA INDEX NAME)



RN 35016-14-9 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-chloro-1,4-diphenyl- (CA INDEX NAME)

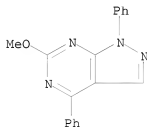


RN 35016-17-2 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidin-6-amine, N,N-dimethyl-1,4-diphenyl- (CA INDEX NAME)



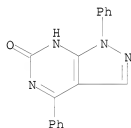
RN 35016-20-7 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-methoxy-1,4-diphenyl- (CA INDEX NAME)



RN 35026-01-8 CAPLUS

CN 6H-Pyrazolo[3,4-d]pyrimidin-6-one, 1,5-dihydro-1,4-diphenyl- (9CI) (CA INDEX NAME)

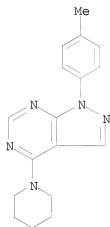


GI For diagram(s), see printed CA Issue.

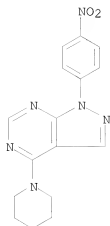
AB When refluxed in AcOH an equimolar mixture of 1-phenyl-3-aminopyrazole and PhCH(NHCONH<sub>2</sub>)<sub>2</sub> (I) gave 34% 1,4-diphenyl-6-oxo-4,5,6,7-tetrahydropyrazolo[3,4-d]pyrimidine (II, R = Ph, R<sub>1</sub> = H) (III) and 10% of its dehydro analog (IV, R = Ph, R<sub>1</sub> = H) (V). V was also prepared from III by its dehydrogenation with Br in AcOH. Prolonged refluxing of V with POC<sub>13</sub> in PhNMe<sub>2</sub> afforded 1,4-diphenyl-6-chloropyrazolo[3,4-d]pyrimidine (VI, R = Ph, R<sub>1</sub> = H, X = Cl) which treated either with MeONa or HNMe<sub>2</sub> gave 6-substituted VI [R = Ph, R<sub>1</sub> = H; X = OMe or NMe<sub>2</sub> (VII)]. VII was also prepared from V by heating with P(O)(NMe<sub>2</sub>)<sub>3</sub>. The other II and IV (R = Me, PhCH<sub>2</sub>, R<sub>1</sub> = H, OMe) were obtained from 1-methyl- or 1-benzyl-3-aminopyrazole and p-MeOC<sub>6</sub>H<sub>4</sub>CH(NHCONH<sub>2</sub>)<sub>2</sub>, resp. An equimolar mixture of 1-phenyl-3-ureidopyrazole (prepared from 1-phenyl-3-aminopyrazole and KNCO in aqueous HCl) and I kept 1 hr at the m.p. afforded 41% 2,4-diphenyl-6-oxo-4,5,6,7-tetrahydropyrazolo[3,4-d]pyrimidine (VIII) and 10% 2,4-diphenyl-6-oxo-6,7-dihydropyrazolo[3,4-d]pyrimidine (IX). IX was also

prepared from VIII by dehydrogenation with chloranil in boiling xylene.

L14 ANSWER 78 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1969:96063 CAPLUS  
 DOCUMENT NUMBER: 70:96063  
 ORIGINAL REFERENCE NO.: 70:17933a,17936a  
 TITLE: Purine analogs. I. Status of Hueckel molecular  
 orbital calculations as predictors of proton shifts,  
 basic strengths, and reactivity  
 AUTHOR(S): Lynch, Brian M.; Robertson, Allan J.; Webb, John G. K.  
 CORPORATE SOURCE: Saint Francis Xavier Univ., Antigonish, NS, Can.  
 SOURCE: Canadian Journal of Chemistry (1969), 47(7), 1129-38  
 CODEN: CJCHAG; ISSN: 0008-4042  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 IT 23000-48-8P 23000-50-2P 23000-51-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 23000-48-8 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-piperidino-1-p-tolyl- (8CI) (CA INDEX  
 NAME)

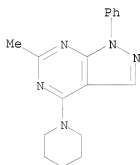


RN 23000-50-2 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-(p-nitrophenyl)-4-piperidino- (8CI) (CA  
 INDEX NAME)



RN 23000-51-3 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-methyl-1-phenyl-4-piperidino- (8CI) (CA INDEX NAME)



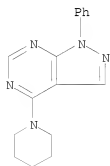
IT 23000-46-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with piperidine)

RN 23000-46-6 CAPLUS

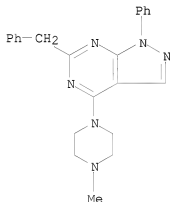
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-phenyl-4-(1-piperidinyl)- (CA INDEX NAME)



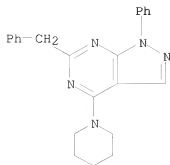
AB A detailed series of M.O. calcns. based on the Hueckel M.O. method was made for the various possible ionic species of purine, pyrazolo[3,4-d]pyrimidine,  $\nu$ -triazolo[4,5-d]pyrimidine, and pyrazolo[3,4-b]pyridine.  $\pi$ -Electron ds. and localization and delocalization energies for nucleophilic substitution were derived. The results are compared with the observed proton chemical shifts in the conjugate acids of these mols. with the relative rates of nucleophilic piperidinodehalogenations in the neutral mols. and with the ionization consts. It is possible to reconcile the calcns. with exptl. results for the various positions within a six-membered ring, but positions in six- and five-membered rings cannot be directly compared. The electron ds. seem to be of little value in correlating the observed ionization patterns of purines and their analogs.

ACCESSION NUMBER: 1964:440466 CAPLUS  
 DOCUMENT NUMBER: 61:40466  
 ORIGINAL REFERENCE NO.: 61:7025b-e  
 TITLE: Pyrazolo[3,4-d]pyrimidines  
 PATENT ASSIGNEE(S): CIBA Ltd.  
 SOURCE: 6 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 937725		19630925	GB 1961-17106	19610510
PRIORITY APPLN. INFO.:			CH	19600511
IT 96267-34-4P, 1H-Pyrazolo[3,4-d]pyrimidine, 6-benzyl-4-(4-methyl-1-piperazinyl)-1-phenyl- 96368-88-6P, 1H-Pyrazolo[3,4-d]pyrimidine, 6-benzyl-1-phenyl-4-piperidino-				
RL: PREP (Preparation)				
(preparation of)				
RN	96267-34-4 CAPLUS			
CN	1H-Pyrazolo[3,4-d]pyrimidine, 6-benzyl-4-(4-methyl-1-piperazinyl)-1-phenyl- (7CI) (CA INDEX NAME)			



RN 96368-88-6 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 6-benzyl-1-phenyl-4-piperidino- (7CI) (CA INDEX NAME)



GI For diagram(s), see printed CA Issue.

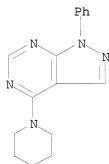
AB The title compds. (I) were prepared by treating I with  $N_2H_4$ ,  $NH_3$ , or an aliphatic amine. A mixture of 15 g. 1-phenyl-4-hydroxy-6-benzylpyrazolo[3,4-d]pyrimidine and 100 ml.  $POCl_3$  was refluxed for 6 hrs. Excess  $POCl_3$  was evaporated, the residue dissolved in  $CHCl_3$  and extracted with  $H_2O$  and  $NaHCO_3$  solution

The  $CHCl_3$  was then evaporated to give I (R = Ph,  $R_1$  = H,  $R_2$  = Cl,  $R_3$  = benzyl) (II), m.  $90-1^\circ$  ( $CHCl_3$ -ligroine). II (7 g.) and 25 g.  $Me_2NH$  in 50 ml. EtOH were heated in an autoclave for 7 hrs. at  $100^\circ$  to give I (R = Ph,  $R_1$  = H,  $R_2$  =  $Me_2N$ ,  $R_3$  = benzyl), m.  $121-2^\circ$  (EtOH). Similarly prepared were the following I (R,  $R_1$ ,  $R_2$ ,  $R_3$ , recrystallization solvent, and m.p. given): iso-Pr, H,  $Me_2N$ , benzyl, ligroine,  $117-18^\circ$ ; iso-Pr, H,  $H_2NNH$ , benzyl, EtOH,  $136-7^\circ$ ; Ph, H, piperidino, benzyl, EtOH,  $116-18^\circ$ ; Ph, H, 4-methyl-1-piperazinyl, benzyl, EtOH,  $122^\circ$ ; iso-Pr, H, piperidino, Ph, ligroine,  $127.5-8.5^\circ$ ; iso-Pr, H, Et $_2N$ , Ph, Et $_2O$ ,  $104-5^\circ$ . Prepared similarly to II was I (R = iso-Pr,  $R_1$  = H,  $R_2$  = Cl,  $R_3$  = Ph), m.  $106-7^\circ$ . A ground mixture of 2-isopropyl-3-aminopyrazole-4-carboxamide and benzamide was heated for 10 hrs. at  $270^\circ$ . The mixture was dissolved in 2N NaOH, filtered and the filtrate brought to pH 6 with 5N HCl to give I (R = iso-Pr,  $R_1$  = H,  $R_2$  = OH,  $R_3$  = Ph), m.  $256-8^\circ$  (EtOH). I are useful as coronary dilators.

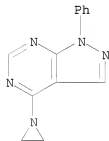


ACCESSION NUMBER: 1962:456317 CAPLUS  
 DOCUMENT NUMBER: 57:56317  
 ORIGINAL REFERENCE NO.: 57:11211b-h  
 TITLE: Derivatives of pyrazolo[3,4-d]pyrimidines  
 INVENTOR(S): Druey, Jean; Schmidt, Paul  
 PATENT ASSIGNEE(S): Ciba Pharmaceutical Products, Inc.  
 SOURCE: 6 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

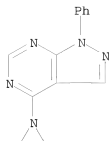
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2965043		19601220	US 1957-692374	19571025
PRIORITY APPLN. INFO.:			CH	19560210
IT 23000-46-6P,				
1H-Pyrazolo[3,4-d]pyrimidine, 1-phenyl-4-piperidino-				
98018-37-2P, 1H-Pyrazolo[3,4-d]pyrimidine, 4-(1-aziridinyl)-1-				
phenyl- 106478-63-1P, 1H-Pyrazolo[3,4-d]pyrimidine,				
4-(1-aziridinyl)-1-phenyl-, hydrochloride				
RL: PREP (Preparation)				
(preparation of)				
RN 23000-46-6 CAPLUS				
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-phenyl-4-(1-piperidinyl)-				(CA INDEX NAME)



RN 98018-37-2 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(1-aziridinyl)-1-phenyl- (CA INDEX NAME)



RN 106478-63-1 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(1-aziridinyl)-1-phenyl-, hydrochloride



## ● HCl

AB For pharmaceutical testing, a series of I were prepared. Thus, to 17 EtOCH<sub>2</sub>C(CN)CO<sub>2</sub>Et (II) in 100 by volume EtOH was added to 10.8 PhNHNH<sub>2</sub> in 50 parts by volume EtOH, the mixture boiled 2 hrs., evaporated to dryness, the residue decolorized with animal C in EtOAc, the mixture filtered, and cooled to precipitate 2-phenyl-3-amino-4-carbethoxypyrazole (III), m. 99-101°. III (12) and 40 parts by volume H<sub>2</sub>NCHO were heated 8 hrs. at 200-10°, the mixture cooled, filtered, the precipitate dissolved in 2N NaOH, decolorized with animal C, and the pH adjusted to 3 with 2N HCl to precipitate I (R = OH,

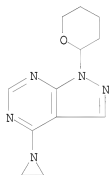
R' = Ph) (IV), m. 286-8°. IV (8) was boiled with 40 parts by volume POC13 2 hrs., the POC13 evaporated, the residue poured over ice, the pH adjusted to 8 with 2N NaOH, the solution extracted with C<sub>6</sub>H<sub>6</sub>, and the C<sub>6</sub>H<sub>6</sub> evaporated

to give I (R = Cl, R' = Ph) (V), m. 125-6° (boiling ligroine). V (23) and 100 parts by volume liquid NH<sub>3</sub> were heated 6 hrs. in a sealed tube at 120 and the NH<sub>3</sub> evaporated to give I (R = NH<sub>2</sub>, R' = Ph), m. 205-6° (CH<sub>2</sub>Cl<sub>2</sub>); HCl salt m. 23940°. Similarly were prepared I (R, R', m. p., and m. p. of HCl salt given): Me<sub>2</sub>N, Ph, 123-4° (boiling ligroine), 218-20°; Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>NH, Ph, -, 141-3° (EtOAc); 2-furfurylamino, Ph, 158-60° (boiling ligroine), 201-3°; MeO, Ph, 115-16° (ligroine), -; HS, Ph, 264-5° (EtOH), -; H<sub>2</sub>NNH, Ph, 180-1°, 209-10°; OH, p-ClC<sub>6</sub>H<sub>4</sub>, did not m. 300°, -; Cl, p-ClC<sub>6</sub>H<sub>4</sub>, 133-5° (boiling CCl<sub>4</sub>), -; Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CHMeNH, Ph, - (b0.1 238-40°), -; piperidino, Ph, 110-12° (CCl<sub>4</sub>-petr. ether), -; HONH, Ph, 170-2° (EtOH), -; H<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>NH, Ph, -, 268-70°; and aziridino, Ph, 124-5° (petr. ether), 284-5°. IV (8.2) in a solution of 0.9 Na by volume in anhydrous EtOH was stirred and heated 3 hrs., 4.5 Me<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>Cl added, the mixture refluxed 5 hrs., evaporated to dryness in vacuo, 100 parts by volume

H2O added, and the mixture filtered to give I (R = Me<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>O, R' = Ph). m. 159-1° (ligroine); HCl salt m. 247-9°. III was similarly condensed with urea to give 1-phenyl-4,6-dihydroxypyrazolo[3,4-d]pyrimidine (VI); HCl salt m. 297-9°. V was hydrogenated in EtOH over Pd-C to absorb 2 moles H and form 1-phenyl-2,3-dihdropyrazolo[3,4-d]pyrimidine; HCl salt m. 200-1°. By starting with (NC)<sub>2</sub>C:CHOEt was similarly prepared 2-phenyl-3-amino-4-cyanopyrazole, m. 135-7° (EtOH), which was hydrolyzed in 2N NaOH to the amide (VII), m. 167-8° (EtOH). VII was similarly condensed with urea to give VI. II was similarly condensed with p-ClC<sub>6</sub>H<sub>4</sub>NHNH<sub>2</sub> to give 2-(p-chlorophenyl)-3-

amino-4-carbethoxypyrazole, m. 145-6°.

L14 ANSWER 81 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1962:456277 CAPLUS  
 DOCUMENT NUMBER: 57:56277  
 ORIGINAL REFERENCE NO.: 57:11197c-i,11198a-b  
 TITLE: Potential purine antagonists. XXXII. The synthesis and antitumor activity of certain compounds related to 4-aminopyrazolo[3,4-d]pyrimidine  
 AUTHOR(S): Sutcliffe, Edward Y.; Zee-Cheng, K. Y.; Cheng, C. C.; Robins, Roland K.  
 CORPORATE SOURCE: Arizona State Univ., Tempe  
 SOURCE: Journal of Medicinal & Pharmaceutical Chemistry (1962), 5, 588-607  
 CODEN: JMPCAS; ISSN: 0095-9065  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 OTHER SOURCE(S): CASREACT 57:56277  
 IT 93086-44-3P, 1H-Pyrazolo[3,4-d]pyrimidine, 4-(1-aziridinyl)-1-(tetrahydropyran-2-yl)-  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 93086-44-3 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(1-aziridinyl)-1-(tetrahydropyran-2-yl)-  
 (7CI) (CA INDEX NAME)



AB A series of derivs. of 4-aminopyrazolo[3,4-d]pyrimidines substituted at the 1-position and (or) at the amino group were prepared and tested for antitumor activity against Adenocarcinoma 755. Of the compds. those with a tetrahydrofuryl or tetrahydropyranyl ring at the 1-position were most active. Cold 3N alc. KOH was added slowly to 40 g. cydohexylhydrazine-HCl in 160 ml. absolute EtOH, the pH adjusted to 8, the precipitate filtered off, washed with hot EtOH twice, the filtrates combined, 32 g. ethoxymethylenemalononitrile added slowly, the solution heated on a steam bath 2 hrs., evaporated to dryness, and the residue recrystd. from H2O to give 19.5 g. 5-amino-4-cyano-1-cyclohexylpyrazole (I), m. 108.5-110°. I (10 g.) was dissolved in 80 ml. formamide, refluxed 1.5 hrs., 50 ml. H2O added, the mixture cooled overnight, the precipitate filtered, dissolved in 140 ml. 2N HCl, decolorized, concentrated NH4OH added to pH 8, the mixture cooled, the precipitate filtered off, washed with H2O, and recrystd. from H2O to give 4.6 g. 4-amino-1-cyclohexylpyrazolo[3,4-d]pyrimidine, m. 196-7°. 4-Chloropyrazolo[3,4-d]pyrimidine (II) (5 g.) and 2.5 g. glycine were refluxed 3 hrs. with 50 ml. concentrated NH4OH, the pH adjusted to 4 with concentrated

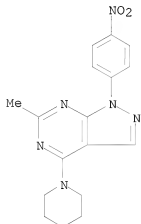
glacial HOAc, filtered, the precipitate recrystd. from dilute NH<sub>4</sub>OH with glacial

HOAc to give 2.1 g. N-[pyrazolo[3,4-d]pyrimidin-4-yl]glycine, decomposing above 215°. II (22 g.) was dissolved in 250 ml. 99% EtOAc, heated with stirring to 35°, 200 mg. p-toluenesulfonic acid added, 12 g. 2,3-dihydropyran added dropwise over 10 min., heating and stirring continued to 45% the solution cooled rapidly to room temperature, washed free

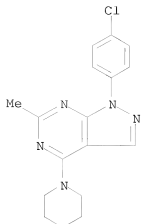
of acid with 4-20 ml. saturated Na<sub>2</sub>CO<sub>3</sub>, followed by 4-20 ml. H<sub>2</sub>O, the exts. dried, the EtOAc removed in vacuo at 60°, and the residue recrystd. from petr. ether to give 10.2 g. 4-chloro-1-(tetrahydropyran-2-yl)pyrazolo[3,4-d]pyrimidine (III), m. 101-2°. Also prepared was 4-chloro-1-(tetrahydro-2-furyl)pyrazolo[3,4-d]pyrimidine. 4-Chloro-1-methylpyrazolo[3,4-d]pyrimidine (12 g.) was added to 100 ml. C<sub>6</sub>H<sub>6</sub> containing 12 ml. Et<sub>3</sub>N, 4 ml. ethylenimine was added, the reaction held at 35° 1 hr., cooled, the precipitate filtered off, the solid extracted with boiling C<sub>6</sub>H<sub>6</sub>, evaporated to dryness in vacuo, and the residue recrystd. from n-heptane to give 7 g. 4-(1-aziridinyl)-1-methylpyrazolo[3,4-d]pyrimidine, m. 141-2°. Prepared similarly were: 4-aziridinyl-1-(tetrahydropyran-2-yl)pyrazolo[3,4-d]pyrimidine, m. 100-2°; 4-dimethylamino-1-(tetrahydro-2-furyl)pyrazolo[3,4-d]pyrimidine, m. 68.5-70.5°; 4-methylamino-1-(tetrahydro-2-furyl)pyrazolo[3,4-d]pyrimidine, m. 180-1°; and 4-dimethylamino-1-(tetrahydropyran-2-yl)pyrazolo[3,4-d]pyrimidine, m. 114.5-15.5°. III (5.7 g.) and 250 ml. saturated ammoniacal absolute EtOH at 0° were heated 2.5 hrs. at 130° in a bomb, cooled, 3 g. KOH added, the mixture filtered, evaporated in vacuo at 60° to dryness, and the residue recrystd. from C<sub>6</sub>H<sub>6</sub> to give 2.5 g. 4-amino-1-(tetrahydropyran-2-yl)pyrazolo[3,4-d]pyrimidine, m. 182.5-3.0°. 4-Aminopyrazolo[3,4-d]pyrimidine (1 g.) 30 ml. glacial HOAc, and 4 ml. 30% H<sub>2</sub>O<sub>2</sub> were stirred 3 days at room temperature, 200 mg. 5% Pd-C added, stirred 1 day, filtered, the solvent removed in vacuo at 60°, and the residue recrystd. from H<sub>2</sub>O to give 0.5 g. 4-aminopyrazolo[3,4-d]pyrimidine 5-N-oxide, m. above 300°. 4-Dimethylaminopyrazolo[3,4-d]pyrimidine (10 g.), 77 ml. MeOH, 34 ml. 2N NaOH and 9.5 g. MeI were refluxed 2.25 hrs., the solution evaporated in vacuo

on a steam bath, the residue dissolved in 77 ml. 10% KOH, filtered, extracted with 3 200-ml. and 3 100-ml. portions of CHCl<sub>3</sub>, the exts. dried overnight, the CHCl<sub>3</sub> removed in vacuo, and the residue recrystd. from heptane to give 3.4 g. 4-dimethylamino-1-methylpyrazolo[3,4-d]pyrimidine, m. 129-9.5°. The insol. residue from the recrystn. solvent was crystallized from toluene, and recrystd. from C<sub>6</sub>H<sub>6</sub> to give 0.2 g. 4-dimethylamino-2-methylpyrazolo[3,4-d]pyrimidine, m. 194-4.5°.

L14 ANSWER 82 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
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RN 107523-46-6 CAPLUS  
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 (6CI) (CA INDEX NAME)



GI For diagram(s), see printed CA Issue.  
 AB cf. C.A. 52, 13741h. A synthesis of 6-alkyl-4-hydroxypyrazolo [3,4-d]pyrimidines,  $R_1N.N:CH.C:C.N:CR_2.N:COH$  (I) was devised from the corresponding 5-acylamino-4-cyanopyrazoles,  $R_3CONHC:C(CN).CR_2:N.NR_1$  (II) which were in turn prepared from 5-amino-4-cyanopyrazoles,  $R_1N.N:CH.C(CN):CNH_2$  (III). Evidence was presented to show that the 5-acylaminopyrazole-4-carboxamide is an intermediate in this cyclization. Chlorination of I yielded the corresponding 6-alkyl-4-chloropyrazolo [3,4-d]pyrimidines,  $R_1N.N:CH.C:C.N:CR_2.N:CCl$  (IV). Nucleophilic displacement of the Cl in IV resulted in the preparation of a large number of 6-alkylpyrazolo[3,4-d]pyrimidines,  $R_1N.N:CH.C:C.N:CR_2.N:CNR_4R_5$  (V). III ( $R_1 = 3-Me$ ) (80 g.) and 250 ml.  $Ac_2O$  refluxed 10 hrs., excess  $Ac_2O$  distilled in vacuo, the sirupy substance poured into 30 ml.  $C_6H_6$ , stirred several min., and crystallized gave 89 g. II ( $R_1 = R_2 = H$ ,  $R_3 = Me$ ), crystals from  $H_2O$ . Similarly II ( $R_1 = R_3 = Me$ ,  $R_2 = H$ ) was prepared and the product recrystd. from  $H_2O$  to a white powder. III ( $R_1 = Ph$ ) (150 g.) treated 19 hrs. under reflux with 200 ml.  $Ac_2O$ , excess solvent removed, the residue treated with a small amount of  $C_6H_6$ , and Skellysolve (b.  $60^\circ$ ), and the product isolated gave 171 g. II ( $R_1 = Ph$ ,  $R_2 = H$ ,  $R_3 = Me$ ) crystallized from  $H_2O$ . The following II were thus prepared ( $R_1$ ,  $R_2$ ,  $R_3$ , m.p., % yield, and recrystn. solvent given):  $H$ ,  $H$ ,  $Me$ ,  $221-2^\circ$ , 76,  $H_2O$ ;  $Me$ ,  $H$ ,  $Me$ ,  $210-11^\circ$ , 72,  $H_2O$ ;  $Ph$ ,  $H$ ,  $Me$ ,  $155-6^\circ$ , 92,  $H_2O$ ;  $o-ClC_6H_4$ ,  $H$ ,  $Me$ ,  $175-5.5^\circ$ , 82, alc.,  $H_2O$ ;  $p-ClC_6H_4$ ,  $H$ ,  $Me$ ,  $173-5^\circ$ , 96, alc,  $H_2O$ ;  $p-BrC_6H_4$ ,  $H$ ,  $Me$ ,  $175-5^\circ$  (sic), 98, alc.,  $H_2O$ ;  $p-O_2NC_6H_4$ ,  $H$ ,  $Me$ ,  $198-200^\circ$ , 95, alc.,  $H_2O$ ;  $p-MeC_6H_4$ ,  $H$ ,  $Me$ ,  $128^\circ$ , 96, alc.,  $H_2O$ ;  $AcOCH_2CH_2$ ,  $H$ ,  $Me$ ,  $155-7^\circ$ , 81, alc. II ( $R_1 = Ph$ ,  $R_2 = H$ ,  $R_3 = Me$ ) (30 g.) added at  $15-20^\circ$  to 120 ml. concentrated  $H_2SO_4$ , the clear solution stirred 0.5 hr., then poured onto 1 kg. ice, neutralized with concentrated  $NH_4OH$ , the solid collected, washed, dried, and recrystd. from  $C_6H_6$  and  $MeOH$  gave 20 g. 5-amino-1-phenylpyrazole-4-carboxamide (VI), m.  $172-5^\circ$ , identical with the product obtained from the hydrolysis of 5-amino-4-cyano-1-phenylpyrazole. VI (20 g.) and 200 ml.  $Ac_2O$  refluxed 15 hrs., and purification gave 15 g. 6-methyl-4-oxo-1-phenylpyrazolo [3,4-d]-5,7-oxazine (VII), m.  $184.5-5.5^\circ$  (sublimed at  $145^\circ$ ) ( $C_6H_6-C_7H_{16}$ ). VII (2.5 g.) kept 2 hrs. at room temperature with 200 ml.  $H_2O$  and 2 g.  $KOH$ , heated 10 hrs., acidified, and the precipitate collected gave 2 g. 5-acetamido-1-phenylpyrazole-4-carboxylic acid (VIII), m.  $201-2^\circ$  ( $AcOH$ ), readily lost  $CO_2$  on

heating. The 5-acetylamido group was retained in warm alkaline solution but hydrolyzed readily in cold acidic medium. VII (2 g.) left 0.5 hr. at room temperature with 100 ml. alc. NH<sub>3</sub>, heated briefly until a solid product precipitated, and the product collected gave 5-acetamido-1-phenylpyrazole-4-carboxamide (IX), m. 301-2°, relatively unstable. The m.p. of IX was the same as that for I (R<sub>1</sub> = Ph, R<sub>2</sub> = Me) and was undepressed in mixed m.p. The ultraviolet absorptions for IX at 230 mμ and for I at 233 and 269 mμ, were different. Thus IX cyclized at elevated temps. during the m.p. determination I were prepared by the following method. II (R<sub>1</sub> = R<sub>2</sub> = H, R<sub>3</sub> = Me) (1.5 g.); 7 ml. 10% KOH, and 15 ml. 3% H<sub>2</sub>O<sub>2</sub> warmed 0.5 hr. at 70-5°, the mixture acidified, the solid collected, and reprecipitated with dilute KOH and AcOH gave 1.1 g. I (R<sub>1</sub> = H, R<sub>2</sub> = Me). II (R<sub>1</sub> = R<sub>3</sub> = Me, R<sub>2</sub> = H) (121 g.) warmed 10 hrs. at 70° with 1500 ml. 3% H<sub>2</sub>O<sub>2</sub> and 400 ml. 10% KOH gave 103 g. I (R<sub>1</sub> = R<sub>2</sub> = Me), needles, sublimed at 180°. II (R<sub>1</sub> = Ph, R<sub>2</sub> = H, R<sub>3</sub> = Me) (14.5 g.) in 5 g. KOH and 200 ml. 3% H<sub>2</sub>O<sub>2</sub> warmed 5 hrs. at 70-5° and acidified gave 14 g. crude I (R<sub>1</sub> = Ph, R<sub>2</sub> = Me), m. 298-300°. IX (1 g.) heated 20 min. at 70° with 100 ml. 10% KOH, then acidified, the solid collected and recrystallized gave 0.8 g. product identical with that from the preceding experiment I (R<sub>1</sub> = R<sub>2</sub> = Me) (25 g.) and 400 ml. POC1<sub>3</sub> refluxed 2 hrs., excess solvent removed, the sirup poured onto 1 kg. ice, the suspension left 15 min., extracted with CHCl<sub>3</sub>, dried, solvent removed at room temperature, and the solid isolated gave 24 g. IV (R<sub>1</sub> = R<sub>2</sub> = Me) as needles. I (R<sub>1</sub> = H, R<sub>2</sub> = Me) (50 g.) refluxed 2 hrs. with 140 ml. PhNMe<sub>2</sub> and 1 l. POC1<sub>3</sub>, excess POC1<sub>3</sub> removed, the residue poured on ice, and extracted with Et<sub>2</sub>O gave 35 g. IV (R<sub>1</sub> = H, R<sub>2</sub> = Me), unstable. I (R<sub>1</sub> = p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, R<sub>2</sub> = Me) (20 g.) refluxed 3 hrs. with 250 ml. POC1<sub>3</sub> gave 17.5 g. IV (R<sub>1</sub> = p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, R<sub>2</sub> = Me) as a yellow powder. Preparation of 1-alkyl(aryl)-6-alkyl-4-mercaptopyrazolo[3,4-d]pyrimidines X (R<sub>1</sub> = 1-substituent, R<sub>2</sub> = 6-substituent) was achieved by the following two methods: (method 1) I (R<sub>1</sub> = Ph, R<sub>2</sub> = Me) (11 g.) and 50 g. P<sub>2</sub>S<sub>6</sub> added portionwise during 45 min. to 400 ml. Tetralin (preheated to 165°), the temperature allowed to rise to 185°, then heated 6 hrs. to 190-5°, the solution cooled overnight, filtered, the product dissolved in dilute KOH and precipitated with AcOH gave 5.5 g. X (R<sub>1</sub> = Ph, R<sub>2</sub> = Me); method 2) IV (R<sub>1</sub> = Ph, R<sub>2</sub> = Me) (14 g.) and 14 g. CS(CH<sub>2</sub>)<sub>2</sub> in 120 ml. alc. refluxed 4 hrs., the product collected and washed well with alc. and H<sub>2</sub>O, and the product purified by precipitation from a hot basic solution with AcOH gave 11.5 g. X (R<sub>1</sub> = Ph, R<sub>2</sub> = Me). All the other X were prepared by essentially the same procedure as method 2. 1-Alkyl(aryl)-6-alkyl-4-alkylthiopyrazolo[3,4-d]pyrimidines (XI) (R<sub>1</sub> = 1-substituent, R<sub>2</sub> = 6-substituent, R<sub>3</sub> = S-substituent) were prepared as follows: X (R<sub>1</sub> = R<sub>2</sub> = Me) (13 g.), 40 ml. 4N KOH, 18 g. MeI, and 30 ml. MeOH shaken 0.5 hr. in a separatory funnel, the contents left overnight at 40°, and the solid collected gave 12.5 g. XI (R<sub>1</sub> = R<sub>2</sub> = R<sub>3</sub> = Me). X (R<sub>1</sub> = Ph, R<sub>2</sub> = Me) (1 g.) added to 200 ml. H<sub>2</sub>O containing 15 g. KOH and 21 g. EtI, treated with 100 ml. alc., refluxed 5 hrs., and reduced in volume, until an oily product solidified gave 3 g. XI (R<sub>1</sub> = Ph, R<sub>2</sub> = Me, R<sub>3</sub> = Et). 4-Alkoxy-1-alkyl(aryl)-6-methylpyrazolo[3,4-d]pyrimidines (XII) (R<sub>1</sub> = 1-substituent, R<sub>2</sub> = O-substituent) were prepared as follows: IV (R<sub>1</sub> = p-MeC<sub>6</sub>H<sub>4</sub>, R<sub>2</sub> = Me) (5.5 g.) and 100 ml. alc. left 2 hrs. at room temperature with 2 g. Na in 70 ml. alc., heated 40 min. on the steam bath, and NaCl removed, the filtrate treated with 50 ml. H<sub>2</sub>O, and left overnight in the cold gave 3.1 g. XII (R<sub>1</sub> = p-MeC<sub>6</sub>H<sub>4</sub>, R<sub>2</sub> = Et). Other XII were prepared as above. The following N:CR<sub>2</sub>:N:CR<sub>3</sub>:C:C.NR<sub>1</sub>:N:CH were prepared by the above methods (R<sub>1</sub>, R<sub>2</sub>, R<sub>3</sub>,



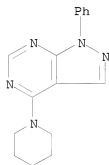
m.p., % yield, and recrystn. solvent given): H, Me, OH, 336-8°, 73.5, AcOH; H, Me, Cl, 140° (decomposition), 70.0, C6H6; H, Me, SH, above 300°, 80, repptd.; H, Et, OH, above 300°, 82, alc., H2O; Me, Me, OH, 277-8°, 72.5, alc., H2O; Me, Me, Cl, 74°, 70.2, C7H16; Me, Me, OMe, 107.5-8.5°, 67.5, MeOH; Me, Me, SH, 264-5°, 98, repptd.; Me, Me, SMe, 74-5°, 90.2, MeOH, H2O; CH2CH2OH, Me, OH, 265-6°, 54.8, H2O; Ph, Me, Cl, 85-6°, 83.5, C7H16; Ph, Me, SH, 268.5°, 83.3, repptd.; Ph, Me, OMe, 121.5-2.0°, -, MeOH; Ph, Me, OEt, 95-5.5°, -, alc.; Ph, Me, SMe, 135-7°, -, MeOH, H2O; Ph, Me, SET, 86-8°, -, alc., H2O; Ph, Et, OH, 295°, 88.5, alc., H2O; Ph, Et, SH, 248-9°, 91.6, repptd.; p-MeC6H4, Me, OH, 298-300°, 93.6, alc., H2O; p-MeC6H4, Me, Cl, 89-91°, 78.1, C7H16; p-MeC6H4, Me, OMe, 121-2°, 81.2, MeOH; p-MeC6H4, Me, OEt, 93-4°, 53, alc.; o-ClC6H4, Me, Cl, 121°, 77.8, C6H14; p-BrC6H4, Me, OH, above 315°, 86.6, alc., H2O; p-BrC6H4, Me, Cl, 130.5-31°, 88.7, C6H14; p-ClC6H4, Me, OH, above 310°, 94.5, alc., H2O; p-ClC6H4, Me, Cl, 129°, 82.6, C7H16; p-ClC6H4, Me, SH, above 305°, 75.2, repptd.; p-O2NC6H4, Me, OH, above 310°, 90, repptd.; p-O2NC6H4, Me, Cl, 184°, 82, PhMe. V were prepared by the following methods: (method A) IV (R1 = H, R2 = Me) (10 g.) and 120 ml. alc. NH3 heated 8 hrs. in a bomb at 160°, the product evaporated to dryness, the residue refluxed with dilute HCl, the solution treated with C, filtered, and the product repptd. with NH4OH, filtered, and recrystd. gave 6.5 g. V (R1 = R4 = R5 = H, R2 = Me); (method B) the above IV (5 g.) added to 7 g. BuNH2, and 120 ml. alc. and the mixture refluxed 7 hrs. gave 3 g. V (R1 = R4 = H, R2 = Me, R5 = Bu). IV (R1 = Ph, R2 = Me) (5 g.) refluxed 40 min. with 8 g. p-ClC6H4NH2 and 75 ml. alc. and the mixture filtered after cooling 3 hrs. in an ice bath gave 6.2 g. crude V (R1 = Ph, R2 = Me, R4 = H, R5 = p-ClC6H4). IV (R1 = p-ClC6H4, R2 = Me) (9 g.) refluxed on a steam bath to near dryness with 160 ml. alc. containing 10 g. PhCH2CH2NH2 and the residue added to MeOH gave 11 g. V (R1 = p-ClC6H4, R2 = Me, R4 = H, R5 = CH2CH2Ph); (method C) IV (R1 = R2 = Me) (5.5 g.), 5.5 g. furfurylamine, and 200 ml. alc. heated 8 hrs. on a steam bath, then evaporated, the residue stirred with 30 ml. 10% KOH, the alkaline solution decanted, the sirup refluxed 2 hrs. with 100 ml. C6H6, and

the

solution, filtered and evaporated to dryness gave 4 g. V (R1 = R2 = Me, R4 = H, R5 = furfuryl as white needles. IV (R1 = Ph, R2 = Et) (13 g.) in 150 ml. alc. treated slowly with 13 g. PhCH2NH2 in 50 ml. alc., the mixture refluxed 12 hrs., the solvent removed, and the product treated with C6H6 and several drops MeOH, and refrigerated gave 8 g. V (R1 = Ph, R2 = Et, R4 = H, R5 = CH2Ph). The following V were prepared by these methods (R1, R2, R4, R5, m.p., method of preparation, % yield, and recrystn. solvents given): H, Me, H, H, above 300°, A, 73, alc., H2O; H, Me, H, Et, 273-4°, B, 56, alc.; H, Me, H, Pr, 220-2°, B, 49.1, alc.; H, Me, H, CH2Ph, 241°, B, 87.2, alc.; H, Me, H, furfuryl, 243-4°, C, 59, alc.; Me, Me, H, H, 251-2°, A, 90, alc., H2O; Me, Me, H, Me, 136-8°, B, 77.2, H2O; Me, Me, H, Et, 131.5-2.0°, C, 66.9, PhMe, C7H16; Me, Me, H, CH2Ph, 180-2°, B, 83, alc.; Me, Me, H, furfuryl, 140-1.5°, C, 54.6, alc.; Me, Me, H, o-ClC6H4, 223.5-4.0°, B, 60, alc.; Me, Me, H, p-ClC6H4, 231.5°, B, 67, alc., H2O; Me, Me, H, p-MeC6H4, 224-5.5°, B, 60, alc.; Me, Me, H, p-MeC6H4, 225-7°, B, 74.7, alc.; Me, Me, H, 2,6-Et2C6H3, 218-18.5°, B, 48.5, alc.; Me, Me, H, NH2, 259-60°, B, 87.3, alc.; Ph, Me, H, H, 287-9°, A, 82.5, alc., H2O; Ph, Me, H, Me, 162-3°, B, 80.2, alc., H2O Ph, Me, Me, Me, 117-17.5°, C, 82.5, alc.; Ph, Me, H, Et, 86°, B, 87.2, alc.; Ph, Me, Et, Et, 66-8°, C, 83, alc.; Ph, Me, H, iso-Pr 143-4°, B, 86, alc., H2O; Ph, Me, H, tert-Bu,

175-70°, C, 61, alc., H<sub>2</sub>O; Ph, Me, H, CH<sub>2</sub>CH<sub>2</sub>NEt<sub>2</sub>, 159-60°, C, 49.1, C<sub>7</sub>H<sub>16</sub>; Ph, Me, CH<sub>2</sub>Ph, H, 187-8°, B, 92, alc.; Ph, Me, H, furfuryl, 153-4.5°, C, 56.2, PhMe, C<sub>7</sub>H<sub>16</sub>; Ph, Me, H, Ph, 262-3°, B, 50.5, EtOCH<sub>2</sub>CH<sub>2</sub>OH; Ph, Me, H, m-BrC<sub>6</sub>H<sub>4</sub>, 215-17°, B, 68, alc.; Ph, Me, H, o-ClC<sub>6</sub>H<sub>4</sub>, 175-6°, B, 51.3, alc.; Ph, Me, H, m-ClC<sub>6</sub>H<sub>4</sub>, 192-3°, B, 90, alc.; Ph, Me, H, p-ClC<sub>6</sub>H<sub>4</sub>, 226-6.5°, B, 82, alc., H<sub>2</sub>O; Ph, Me, H, 2,6-Et<sub>2</sub>C<sub>6</sub>H<sub>3</sub>, 189-90°, B, 71.2, alc.; Ph, Me, H, NH<sub>2</sub>, 243-4°, B, 80.1, C<sub>5</sub>H<sub>5</sub>N; Ph, Me, H, NPh, 240-1°, B, 47.5, C<sub>5</sub>H<sub>5</sub>N; Ph, Et, Me, Me, 90.5-1.0°, B, 55.5, alc.; Ph, Et, H, tert-Bu, 148-8.5°, C 73.3, alc. (sublimed); Ph, Et, H, CH<sub>2</sub>Ph, 129-9.5°, C, 48.5, C, 48.5, C<sub>6</sub>H<sub>6</sub>, alc.; Ph, Et, H, o-ClC<sub>6</sub>H<sub>4</sub>, 168-8.5°, B, 71.5, EtOCH<sub>2</sub>CH<sub>2</sub>OH; Ph, Et, H, m-ClC<sub>6</sub>H<sub>4</sub>, 187-9°, B, 74, alc.; Ph, Et, H, p-ClC<sub>6</sub>H<sub>4</sub>, 208.5-9.5°, B, 87.8, EtOCH<sub>2</sub>CH<sub>2</sub>OH; Ph, Et, H, o-MeC<sub>6</sub>H<sub>4</sub>, 175-6°, B, 75.5, alc.; Ph, Et, H, m-MeC<sub>6</sub>H<sub>4</sub>, 169.5°, B, 58, alc.; Ph, Et, H, p-MeC<sub>6</sub>H<sub>4</sub>, 199-200°, B, 78.6, alc.; Ph, Et, H, 2,5-Cl<sub>2</sub>C<sub>6</sub>H<sub>3</sub>, 181-3°, B, 42.1, alc.; Ph, Et, H, 2,6-Et<sub>2</sub>C<sub>6</sub>H<sub>3</sub>, 191-1.5°, B, 38, alc.; Ph, Et, H, NH<sub>2</sub>, 198-9°, B, 87.5, alc.; p-MeC<sub>6</sub>H<sub>4</sub>, Me, H, H, 296.5-8.0°, A, 75.7, alc.; p-MeC<sub>6</sub>H<sub>4</sub>, Me, H, Me, 181-2.5°, B, 86, MeOH, H<sub>2</sub>O; p-MeC<sub>6</sub>H<sub>4</sub>, Me, Me, Me, 149-51°, B, 82.2, alc.; p-MeC<sub>6</sub>H<sub>4</sub>, Me, H, Et, 144-6°, B, 80, alc., H<sub>2</sub>O; p-MeC<sub>6</sub>H<sub>4</sub>, Me, H, CH<sub>2</sub>CH<sub>2</sub>NEt<sub>2</sub>, 165°, C, 62.8, PhMe, C<sub>7</sub>H<sub>16</sub>; p-MeC<sub>6</sub>H<sub>4</sub>, Me, H, o-ClC<sub>6</sub>H<sub>4</sub>, 219-21°, B, 76.5, C<sub>5</sub>H<sub>5</sub>N; p-MeC<sub>6</sub>H<sub>4</sub>, Me, H, m-BrC<sub>6</sub>H<sub>4</sub>, 218-20°, B, 63.5, alc.; o-ClC<sub>6</sub>H<sub>4</sub>, Me, H, H, 294.5-9.5°, A, 71.8, alc.; o-ClC<sub>6</sub>H<sub>4</sub>, Me, Me, Me, 152-3°, C, 77.7, alc.; o-ClC<sub>6</sub>H<sub>4</sub>, Me, H, o-ClC<sub>6</sub>H<sub>4</sub>, 196-8°, B, 63, alc.; p-BrC<sub>6</sub>H<sub>4</sub>, Me, Et, Et, 123-4°, B, 51.6, EtOCH<sub>2</sub>CH<sub>2</sub>OH, H<sub>2</sub>O; p-ClC<sub>6</sub>H<sub>4</sub>, Me, H, H, above 300°, A, 36, alc.; p-ClC<sub>6</sub>H<sub>4</sub>, Me, H, Me, 218-19°, B, 57.2, alc.; H<sub>2</sub>O; p-ClC<sub>6</sub>H<sub>4</sub>, Me, H, iso-PrO(CH<sub>2</sub>)<sub>3</sub>, 109-10°, B, 51.1, MeOH, H<sub>2</sub>O; p-ClC<sub>6</sub>H<sub>4</sub>, Me, (R<sub>4</sub>R<sub>5</sub> = ) (CH<sub>2</sub>)<sub>5</sub>, 127.5-8.5°, B, 61.3, alc., H<sub>2</sub>O; p-ClC<sub>6</sub>H<sub>4</sub>, Me, H, CH<sub>2</sub>Ph, 214°, B, 93.3, EtOCH<sub>2</sub>CH<sub>2</sub>OH; p-ClC<sub>6</sub>H<sub>4</sub>, Me, H, CH<sub>2</sub>CH<sub>2</sub>Ph, 175-6°, B, 60.1, alc.; p-ClC<sub>6</sub>H<sub>4</sub>, Me, H, o-ClC<sub>6</sub>H<sub>4</sub>, 221-2°, B, 62.0, C<sub>5</sub>H<sub>5</sub>N, p-ClC<sub>6</sub>H<sub>4</sub>, Me, H, m-ClC<sub>6</sub>H<sub>4</sub>, 222-3°, B, 85.5, EtOCH<sub>2</sub>CH<sub>2</sub>OH; p-ClC<sub>6</sub>H<sub>4</sub>, Me, H, p-ClC<sub>6</sub>H<sub>4</sub>, 239-9.5°, B, 88, C<sub>5</sub>H<sub>5</sub>N; p-ClC<sub>6</sub>H<sub>4</sub>, Me, H, m-BrC<sub>6</sub>H<sub>4</sub>, 230-2°, B, 74.2, C<sub>5</sub>H<sub>5</sub>N; p-ClC<sub>6</sub>H<sub>4</sub>, Me, H, 2,5-Cl<sub>2</sub>C<sub>6</sub>H<sub>3</sub>, 200°, B, 71.5, EtOCH<sub>2</sub>CH<sub>2</sub>OH; p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, Me, H, Me, 248-9°, B, 69, alc.; p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, Me, Me, Me, 196°, B, 51.2, alc., H<sub>2</sub>O; p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, Me, H, iso-Pr, 190-2°, B, 81.1, alc.; p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, Me, H, Bu, 147°, B, 66.6, alc.; p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, Me, (R<sub>4</sub>R<sub>5</sub> = ) (CH<sub>2</sub>)<sub>5</sub>, 189-91°, B, 96, C<sub>5</sub>H<sub>5</sub>N; p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, Me, H, CH<sub>2</sub>CH<sub>2</sub>NEt<sub>2</sub>, 145°, B, 91.7, alc., H<sub>2</sub>O; p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, Me, H, o-ClC<sub>6</sub>H<sub>4</sub>, 227-8°, B, 43.2, alc.; p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, Me, H, p-ClC<sub>6</sub>H<sub>4</sub>, 278°, B, 87, AcOH. The ultraviolet spectra were given for many of the compds. given above. The screening of these compds. against tumors in mice thus far has not revealed any significant antitumor agents in this series.

L14 ANSWER 83 OF 83 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1956:89217 CAPLUS  
 DOCUMENT NUMBER: 50:89217  
 ORIGINAL REFERENCE NO.: 50:16791a-c  
 TITLE: Chemotherapeutic studies in the heterocyclic series.  
 XIV. Pyrazolo[3,4-d]pyrimidines  
 AUTHOR(S): Schmidt, P.; Druey, J.  
 CORPORATE SOURCE: C I B A, Basel, Switz.  
 SOURCE: Helvetica Chimica Acta (1956), 39, 986-91  
 CODEN: HCACAV; ISSN: 0018-019X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German  
 OTHER SOURCE(S): CASREACT 50:89217  
 IT 23000-46-6P, 1H-Pyrazolo[3,4-d]pyrimidine, 1-phenyl-4-piperidino-  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 23000-46-6 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-phenyl-4-(1-piperidinyl)- (CA INDEX NAME)



AB cf. C.A. 50, 2614d. EtOCH:C(CN)CO<sub>2</sub>Et (I) and N<sub>2</sub>H<sub>4</sub> form either  
 H<sub>2</sub>NNHCH:C(CN)CO<sub>2</sub>Et, m. 89-90°, on standing overnight at room temperature,  
 or Et 3-amino-4-pyrazolecarboxylate (II), m. 102-3°, on refluxing 6  
 hrs. The free acid of II, m. 120°, is decarboxylated to the known  
 3-aminopyrazole, b<sub>11</sub> 146-8°. II with HCONH<sub>2</sub> forms  
 4-hydroxypyrazolo[3,4-d]pyrimidine (III), m. above 350°, previously  
 prepared via a longer series of reactions by Robins (C.A. 50, 13037b). II  
 and urea or thiourea form 4,6-dihydroxy- (IV) and 4-hydroxy-6-  
 mercaptopyrazolo[3,4-d]pyrimidines. I and PhNNH<sub>2</sub> form the  
 2-Ph-substituted II, m. 99-101°, from which the 1-Ph-substituted  
 III and IV, m. 286-8° and 297-8°, resp., are prepared. The  
 following 4-substituted-1-phenylpyrazolo[3,4-d]pyrimidines are reported  
 with no preps. described (substituent and m.p. given): SH, 265-7°;  
 NH<sub>2</sub>, 205-6°; NNNH<sub>2</sub>, 180-1°; NMe<sub>2</sub>, 124-5°;  
 2-furylmethylamino, 158-60°; NH(CH<sub>2</sub>)<sub>2</sub>NEt<sub>2</sub>·HCl, 141-3°; OMe,  
 115-16°; O(CH<sub>2</sub>)<sub>2</sub>NMe<sub>2</sub>, 150-1°; Cl, 126-7°; NC<sub>5</sub>H<sub>10</sub>,  
 113-14°.

=>

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	467.95	830.40
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-66.40	-66.40
STN INTERNATIONAL LOGOFF AT 17:16:51 ON 15 MAY 2008		